ALTERNATING FLOW MODEL FOR DISPERSION IN PACKED BEDS

By

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NOTATION

a_i	constants for Cohen-Metzner porosity correlations
a(j,k)	interfacial area between j-th and k-th radial plugs per unit bed length (equations (20), (22)) (L)
a(s,w)	interfacial area between N-th solid plug and stagnant wall film per unit bed length (L)
A_i	void cross-sectional area of i-th radial plug (L^2)
$\underline{A}_n$	concentration vector for A-half-cell of n-th A/B cell
A*	heat transfer area ratio (equation (27)) (L/L)
At	total tube cross-sectional area (L^2)
Atube	At
B	collection of heat transfer terms (equation (28) or (35))
$\underline{B}_n$	concentration vector for B-half-cell of n-th A/B cell
C	concentration (mol/L^3)
C*	two plug verage concentration (equation 54) (mol/L^3)
$\underline{CA}$	A-half-cell concentration vector equations (74), (75))
$\underline{CB}$	B-half-cell concentration vector (equations (74), (75))
C_p	fluid specific heat (q/M-θ)
d	diameter of cylindrical pellet (equation (28)) (L)
d_i	delay time in i-th radial plug
dp	pellet diameter (L)

Da	axial mass dispersion coefficient (equation (1)) (L^2/t)
De	effective diffusivity of key component in catalyst material (L^2/t)
Dr	radial mass dispersion coefficient (equation (1)) (L^2/t)
Dt	tube diameter (L)
f	friction factor
g	rate constant exponent (equation 52) (θ)
g_c	units conversion factor (e.g. 32.2 ft.-lb_m/lb_f-s^2)
G	mass velocity (M/L^2 - t)
hp	pellet film heat transfer coefficient (q/t-L^2-θ)
hw	wall film heat transfer coefficient (q/t-L^2-θ)
h*	stagment film heat transfer coefficient (equation (33)) (q/t-L^2-θ)
(-ΔH)	heat of reaction (q/mol)
H_i	hydraulic resistance of i-th radial plug
k	reaction rate constant
k_o	rate constant premultiplier (equation (51))
K'	constant for equation (41)
K"	constant for equation (42)
Kw	constant for equation (45)
ℓ	length of cylindrical pellet (equation (46))(L)
L	total vessel length; or, if used in conjunction with catalyst pellet, L = Vp/Sp (L)

m	flow rate exponent (equation (45))
N	total number of radial plugs in any half-cell (or, total number of void plugs in one A/B cell)
N_{axial}	number of repeating A/B cells in a packed bed
Nrad	N
P	general physical property (equations (79), (80)); pressure elsewhere
Qt	total volumetric flow rate (L^3/t)
Qtot	Qt
Q_j	volumetric flow rate through j-th radial plug (L^3/t)
r	radial position (dimensional for equations (1), (19); dimensionless elsewhere)
r_c	intrinsic reaction rate (equation (51)) (mol/t-$L^3_{catalyst}$
$r_{i,j}$	(i,j)-th element of $\underline{\underline{R}}$
$\underline{\underline{R}}$	A-to-B mixing matrix
Rt	tube radius (L)
Rtube	Rt
Re	Reynolds number
R_G	global rate of reaction (mol/t); $R'_G = R_G/z$ (mol/t-L)
Rh	hydraulic radius (L)
s	Laplace variable (1/t)
$S_{i,j}$	(i,j)-th element of $\underline{\underline{S}}$
$\underline{\underline{S}}$	B-to-A mixing matrix
Sp	catalyst pellet surface area (L^3)

Sp'	Sp per unit vessel length (equation (60)), (L)
t	solid temperature (θ)
t_{in}	temperature of solid plug at inner radius (equations (25), (34)), (θ)
t_{out}	temperature of solid plug at outer radius (equation (26)) (θ)
T	fluid temperature (θ)
T*	two-plug average temperature (equation (54)), (θ)
$\underline{TA}$	A-half-cell temperature (equations (74), (75))
$\underline{TB}$	B-half-cell temperature vector (equations (74), (75)
Twall	wall temperature (θ)
u	fluid velocity (L/t)
u'	bed average velocity (L/t)
Vp	catalyst pellet volume (L^3)
w_i	weighting factors for $\underline{\underline{R}}$ and $\underline{\underline{S}}$ (equation (8))
x	radial distance inward from tube wall (units of dp)
Y	parameter group for equation (70)
z	axial coordinate (L)
Z	Ztot
Zc	length of one A/B cell (L)
Ztot	total bed length (L)

Greek

β	proportionality constant
γ	shape factor for hp (equation (50)) (γ = 1.0 for spheres, 1.33 for cylinders)
δ	tube material roughness (L)
ε	bed void fraction (L^3/L^3)
$\underline{\underline{\theta}}_A$	A-half-cell delay time matrix
$\underline{\underline{\theta}}_B$	B-half-cell delay time matrix
λ	effective thermal conductivity (equation (19)) (q/L-t-θ)
λ_s	thermal conductivity of solid packing material (q/L-t-θ)
μ	fluid viscosity (M/L^2-t)
ρ	fluid density (M/L^3)
τ	bed-averaged hold-up time (t)
ϕ	Thiele modulus (equation (52)); or functional form (Table 6)

Subscripts

a	radially averaged value
b	bulk or bed-averaged
base	base case value
c	at bed centerline
h	hydraulic
hi	upper value
in	inlet
int	interstitial
lo	lower value
n	axial cell number
out	outlet
p	particle (except for C_p)
s	solid (packing) material
sup	superficial
t	two or total

Units

L	length
M	mass
q	heat (e.g. cal)
t	time
θ	temperature

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The Alternating Flow Model (AFM) views dispersion in packed beds as a sequence of streamline plugs which must repeatedly split and merge as the bulk fluid traverses the vessel. Thus, the flow in the AFM is ordered, as opposed to the random flow implied by the Fickian analogy.

For mass dispersion only, model parameters arise from a priori consideration of packing geometry. Steady-state and transient data ($5.6 < Dt/dp < 54.4$, $100 < Re_p < 1000$, gases and liquids) show the AFM to surpass the Fickian analogy in most cases. Further, the AFM can describe well the radial velocity profiles in packed beds.

Alternating Flow Model heat transfer parameters wall and pellet film resistances are not a priori functions of packing geometry. Fitting the AFM to steady-state temperature data (air, $5 < Dt/dp < 14$, $2 < Re_p < 1300$, cylindrical and spherical pellets) validates a single correlation of hp versus dp and flow rate and justifies a simple form for correlating hw versus flow rate. Comparison with experiments shows the AFM to equal or surpass the back-fit Fickian analogy.

For reaction, the AFM combines the concepts of simple mass and heat dispersion with the only additional parameters associated directly with the reaction itself (e.g. intrinsic rate expression, heat of reaction, etc.) AFM-predicted conversion and temperature profiles in both wall-cooled and adiabatic reactors differ significantly from those predicted by the Fickian analogy for the given example system. The difference in the models' predictions of reactor stability characteristics can be attributed to their respective radial flow profiles. This implies that the AFM, with its ability to describe this flow behavior, should be further explored as a packed bed reactor design tool.

CHAPTER I
INTRODUCTION

Consider the problem of describing the concentration profile which develops as dye is injected into a clear fluid flowing through a tubular packed bed. After some period of time, the dye concentration will be maximum at the injection point and will decrease as the distance from the injection point increases both radially and axially in the direction of flow. This dye dilution is the simplest case of dispersion in packed beds. If the dye reacts in the bulk fluid or on the pellets, or if the dye adsorbs on the solid surfaces and if heat dispersion accompanies the dispersion of mass, the problem becomes more complex, but a basic understanding of the mass dispersion phenomenon alone is needed before moving up the hierarchy. It is therefore the intent in this paper to present a packed bed dispersion model which is based on the physical behavior of the bulk fluid as it travels around the packing.

Dispersion in packed beds has traditionally been modeled by analogy to Fickian diffusion, e.g., for a constant density fluid

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial z} - Da \frac{\partial^2 C}{\partial z^2} - Dr \frac{1}{r} \frac{\partial}{\partial r}\left[r \frac{\partial C}{\partial r}\right] = 0 \qquad (1)$$

where the axial and radial dispersion coefficients Da and Dr are effective parameters which account for the presence of packing material. It should be noted here that equation (1) can be developed by assuming random motion of particles moving through the vessel (Baron, 1952; Jacques and Vermeulen, 1957; Klinkenberg and Sjenitzer, 1956). The usual procedure for modeling packed beds is to obtain the dispersion coefficients and then to solve (1) either analytically or numerically for the appropriate boundary conditions.

An acceptable dispersion model should at the very least adequately describe the simplest problem of injecting non-reacting dye into a clear stream flowing through a bed packed with non-porous beads. The solution of (1) for the simple dye injection problem predicts backmixing in the steady state (Hiby, 1963) where none is observed experimentally.

Mixing cell models (Deans and Lapidus, 1960; Lapidus and Amundson, 1977; Olbrich et al., 1966) overcome the backmixing problem but predict that concentration wavefronts travel at infinite speed, i.e. any change in inlet concentration is immediately seen at the bed outlet. Experimental observations (Sundaresan et al., 1980) indicate that concentration propogates at a finite speed. Also, no standard technique for sizing the individual mixing cells is available.

A more recent crossflow model (Hinduja, 1977; Hinduja et al., 1980) is based on the concept that the flow around pellets creates two regimes--a stagnant wake behind each pellet and moving streams

travelling between pellets. The wakes are assumed to shed/receive a certain amount of fluid to/from the moving streams and the packing is characterized by a parameter which accounts for the radial distance over which the packing pattern repeats itself. Hinduja (1977) recommends determining the cross-flow characteristic parameters from the correlations of effective Fickian dispersion coefficients. It should also be noted that for the simple dye injection problem, the cross-flow model equations reduce to the Fickian dispersion model.

Other researchers have also proposed stochastic (Schmalzer and Hoelscher, 1971), capillary (Lippert and Schneider, 1979), and probabilistic time-delay models (Buffham, 1971) for packed beds. In addition, the literature provides several reviews of and cautions regarding packed bed models (Aris and Amundson, 1957; Beek, 1962; Bischoff and Levenspiel, 1962; Froment, 1967, 1972; Gunn, 1968; Hiby, 1963; Levenspiel, 1963; Vortmeyer and Winter, 1984).

What, then, are the characteristics of an acceptable packed bed dispersion model? The model should provide the correct steady-state form (axial and radial spreading, no back-mixing, agreement with experimental data) and should predict the correct transient behavior (finite speed of propagation, conservation system) Sundaresan et al., 1980). The model should also properly represent the flow around packing, its solution, analytical or numerical, should be straightforward, and its corresponding parameters should be well-defined. Table 1 indicates that none of the currently available models meet all acceptability criteria.

The objectives here are to present a model which describes the flow in packed beds as a series of alternating annular plugs, the so-called Alternating Flow Model (AFM), and then to develop the corresponding mathematical model. Conceptually, this AFM meets all the criteria set forth in Table 1. Its applicability thus depends on adequate representation of the packing interstices as a regular pattern of concentric annular voids. The second chapter justifies the AFM by physical and other reasoning and the remaining chapters develop the pertinent equations for cases of varying degrees of complexity. As each case in considered, corresponding model parameters will be evaluated. While at first glance the number of parameters may seem quite large, the AFM utilizes an a priori distribution of voids based on the relative size of tube to pellets and on packing geometry, rather than on back-fitting those parameters to experimental data.

First, cases of mass dispersion only, both steady-state and transient, will be considered so that the physical dimensions of the individual plugs can be determined. Next, the case of heat dispersion only will be used to extend the applicability of the AFM and to identify the additional parameters which may be needed to describe energy dispersion. And, finally, because the AFM is particularly applicable to vessels with small tube- to pellet-diameter ratios, equations for combined heat and mass dispersion (i.e., reaction within the catalytic packing) will be presented, since highly exothermic reactions are normally carried out in tubes with a small number of pellets across the tube diameter to facilitate cooling.

Table 1

Dispersion Model Acceptability Criteria

	Fickian	Mixing 1-D	Cell 2-D	Crossflow	AFM
Finite wavefront speed	depends on BC's	No	No	depends on BC's	Yes
Conservation system	depends on BC's	Yes	Yes	depends on BC's	Yes
Radial and axial spreading	if all terms used	No	Yes	Yes	Yes
No back-mixing	depends on BC's & terms	Yes	Yes	depends on BC's & terms	Yes
Agreement with data	if fit disp. coeffs.	for avg. conc.	if fit params	??	Yes
				??	Yes
Easy to solve	depends on BC's etc.	Yes	sec. ODE's	simult. PDE's	Yes
Account for packing	adjust coeffs	-empirical- cell size		uses Fickian coeffs	a-priori based on Dt/dp

CHAPTER II
MASS DISPERSION

Concept and Rationale for Proposed Model

Traditionally, two experiments have been used to characterize mass dispersion in empty tubes: steady-state injection of dye at some point along the centerline axis (as mentioned earlier) and time-dependent variation (e.g., step change or sine wave) in the cross-sectional inlet concentration. The steady-state case results in a parabolic shape profile emanating from the point of injection in the direction of bulk flow whereas the transient case yields the residence time distribution (or the so-called "F-curve," if the input is a step-change) which uses the bulk average outlet concentration as an indication of deviation from plug-flow. General practice, as established by Aris (1956, 1958, 1959) and Taylor (1953, 1954a, 1954b), is then to describe this dispersion behavior by a Fick's Law analog (equation (1)). These axial and radial dispersion coefficients, Da and Dr, (in the form of a dimensionless Peclet Number) are correlated for each of the three flow regimes (laminar, turbulent, transition) (Hoffmann, 1961) in terms of Reynolds and Schmide Numbers. It is generally accepted that use of the dispersion parameters obtained from these correlations together with the numerical or analytical solution of equation (1)

and its corresponding boundary conditions accurately predicts observed concentration profiles and residence time distributions in empty tubes.

If these same two experiments are carried out in a packed bed, similar (but not exactly equivalent) dispersion characteristics are observed (Danckwerts, 1953; Hiby, 1963). Thus, usual practice is to again employ Fick's Law, together with numerical or readily available analytical solutions of equation (1) (Carberry, 1976; Froment and Bischoff, 1979; Wen and Fan, 1975), but to use effective parameters to account for the fact that the tube is partially occupied by packing. Again, the effective Peclet Numbers (both radial and axial) are correlated in terms of Reynolds and Schmide Numbers (Wen and Fan, 1975; see also list of pertinent references in Appendix A). Unlike empty tubes, however, these parameters are not well-correlated; there is much spread in the data. The spread exists within the data of single researchers as well as between average values reported by different researchers. One might attribute this spread in Peclet numbers to several factors:

1. misrepresentation of the Reynolds Number,
2. variations in void fraction,
3. erroneous application of the Fickian analogy.

First, consider calculation of the Reynolds number for a packed bed. While in empty tubes it is the diameter that affects transition from laminar to turbulent flow, there is some doubt as to what length actually characterizes this behavior in packed beds, which have,

essentially, two competing lengths: tube diameter and pellet diameter. Usual practice is to employ the pellet diameter since flow around single spheres is well-documented (Bird et al., 1960). However, it has been suggested that it is not the pellet diameter, per se, which induces turbulence but rather the size of the voids, i.e., interstitial hydraulic radius, through which the fluid moves that dominates flow patterns, and that this hydraulic radius should determine a more correct Reynolds number (Cairns and Prausnitz, 1960; Bird et al., 1960; Schertz and Bischoff, 1969; Ergun, 1952; Ergun and Orning, 1949; Lapin, 1962; Leva, 1947a, 1947b; Leva and Grummer, 1947a; Martin et al., 1951). The hydraulic radius for beds with spherical pellets can be calculated from the bed voidage in two ways:

1. $Rh' = \dfrac{Dt\,\varepsilon}{1.5\,\frac{Dt}{dp}\,(1-\varepsilon) + 2}$ (Cairns and Prausnitz, 1960);

2. $Rh = \dfrac{dp\,\varepsilon}{6(1-\varepsilon)}$ (Bird et al., 1960)

In either case, however, re-plotting the Peclet number in terms of this corrected Reynolds number, i.e., with Rh as the characteristic length, does not significantly reduce the spread. Figure 8 of Cairns and Prausnitz (1960) illustrates this point for the case of Rh'. For the case of Rh consider the relationship between the pellet-

and hydraulic-Reynolds numbers: $Re_h = Re_p \varepsilon/6(1-\varepsilon)$. Since the usual practice is to plot Peclet number versus Reynolds number on logarithmic axes, all data would translate horizontally by the same amount since $\log(Re_h) = \log(Re_p) + \log(\varepsilon/6(1-\varepsilon))$. Given that ε falls within a narrow range, the second term is essentially constant.

Second, although packed beds are inherently non-homogeneous merely by the presence of packing, the void fraction within a bed is not constant throughout but depends on radial position (see Appendix C for list of appropriate references). Thus, although the dispersion parameters, i.e., Peclet numbers, are effectively adjusted to account for that portion of the bed unavailable for flow (and mixing), use of the average bed void fraction to do so can induce errors, since the void fraction, in general, determines the average velocity of equation (1). If velocity varies as a function of radial position, then it follows that the dispersion characteristics should also vary radially. Cohen and Metzner (1981) summarize the radial fluctuations in void fraction in terms of a tri-regional (wall, transition, bulk) equation. Their correlation documents maximum voidage near the tube wall with sinusoidal variations about the average bed voidage whose amplitude decays exponentially as one moves from the wall to the centerline. While voidage variations are thus well-established, the corresponding velocity variations are not. In fact, while one would expect minimum velocity to correspond to maximum cross-sectional area, the converse has been consistently observed

(Carbonell, 1980; Gunn, 1969; Karabelas, et al., 1973; Mickley et al., 1965; Schertz and Bischoff, 1969; Schwartz and Smith, 1953; Standish, 1984; Vortmeyer, 1983; Vortmeyer and Schuster, 1984). This maximum velocity/maximum voidage effect can be attributed to channelling--that more fluid will take the path of least hydraulic resistance, i.e. maximum cross-sectional area. In addition, other researchers (Fahien and Smith, 1955; Edisath et al., 1983; Dorweiler and Fahien, 1959; Oliveros and Smith, 1982) have shown that allowing the individual dispersion coefficients to be functions of radial position improves the accuracy of the Fickian description (equation (1)) of packed beds; Fahien and Smith (1955) showed that the dispersion coefficient also varies axially.

Third, consider the possibility that it may be the model itself, rather than the corresponding parameters, that is in error. Why does the Fickian analogy work so well for empty tubes but present difficulties when applied to packed beds? Some researchers have attributed this to the dubious applicability of the usual boundary conditions to packed beds (Burghardt and Zaleski, 1968; Chen et al., 1983; Choi and Perlmutter, 1976; Deckwer and Mahlmann, 1976; Rasmuson and Neretnieks, 1980; Rasmuson, 1981; Ray et al., 1972; Standart, 1968; Wehner and Wilhelm, 1956), but the key here is to examine the underlying assumption of randomness implied by the application of Fick's Law. It has been shown (Baron, 1952; Jacques and Vermeulen, 1957) that if a particle exhibits random motion, with no preference for direction of travel, as it traverses the length of the vessel, then

statistical analysis will lead to equation (1). The question then arises as to whether the presence of packing within the tube would impose some order to the flow.

Gunn and Pryce (1969) carried out several experiments in packed beds of two types: one with the packing intentionally arranged in a regular pattern and another with random (dumped) packing. Their goal was to compare the applicability of the Fickian analogy to the tanks-in-series model. The initial hypothesis was that the tanks-in-series model should more closely fit the ordered packing arrangement since regular pockets would be available for the formation of perfect mixers, whereas the Fickian analogy should better describe the random packing arrangement. They reasoned that if the parameters associated with each of these models could be fit within reasonable statistical significance, the model itself would be applicable to that particular situation. Their data analysis showed that, within the desired accuracy, the tanks-in-series model parameters could not be fit to either the random or regular packing cases, that the Fickian dispersion parameters could not be fit to the regular array case, and that the Fickian parameters did fit the random packing case. This lends support to the idea that equation (1) may not adequately describe conditions of non-random motion.

In addition, other researchers (Hiby, 1963; Bischoff and McCracken, 1966; Kubo et al., 1979) experimented with time-lapse photography to observe the flow patterns around pellets in packed beds.

Patterns, such as those shown schematically in Figure 1, were consistently observed. The experiment illustrated in Figure 1 is for flow around cylinders between two flat plates. This streamline-split/merge pattern did not break down even as the velocity was increased by two orders of magnitude (Hiby, 1963). This lends support to the idea that the packing arrangement dominates the actual fluid velocity in determining mixing characteristics within packed beds.

How, then, is it possible to use this information to aid the description of dispersion in packed beds? If one draws a vertical axis through the middle of the flat plates illustrated by Figure 1 and then rotates these plates about that axis, the void and occupied channels become void and occupied annuli as shown in Figure 2. As the fluid flows through this sequence of void-full annular cells it alternately splits and merges; hence, the name Alternating Flow Model (AFM). The basic premise of this work, then, is that this AFM approximation, developed solely from observations of packed bed flow behavior, accurately describes not only the flow, but also the dispersion behavior in packed beds. Further, the resulting equations can be solved in a straightforward manner and the corresponding physical parameters can be determined a priori, as opposed to being back-fit to laboratory data.

General Description of Alternating Flow Model

The Alternating Flow Model presumes that flow through a packed bed can be described by an axially repeating series of cells as shown in Figure 2, and that the fluid moving through each void space

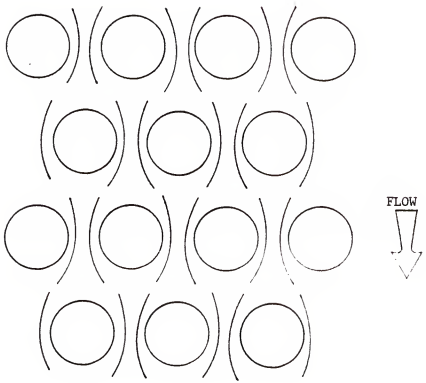


Figure 1: Schematic Representation of Flow Patterns in Packed Beds

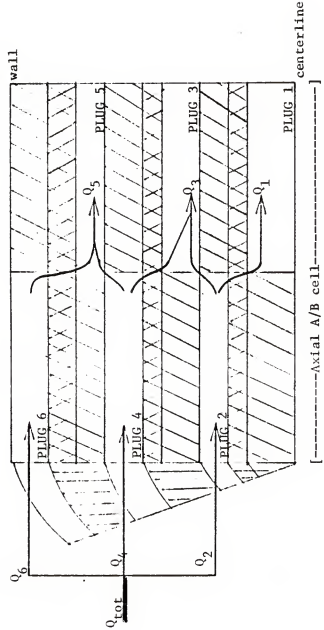


Figure 2: One AFM Repeating A/B cell, $N_{rad}=6$

exhibits plug flow behavior. Thus, dispersion is achieved by repeated splitting and merging of these fluid plugs as the bulk fluid traverses the length of the bed.

Note that the underlying assumption here is that the packing exerts a great influence on the flow pattern, i.e., the packing imposes order on the flow. Hence, the randomness assumption inherent in the Fickian analogy no longer holds. One might argue that if the tube to pellet diameter ratio, Dt/dp, is large enough, the choice of pathways available to a particle as it traverses the bed will be sufficiently large to validate the randomness assumption. One might intuitively justify this argument by pointing out the large number of possible arrangements the pellets can assume as they are packed in the tube. Consider, however, what happens as Dt/dp decreases; the number of possible arrangements also decreases. For example, if Dt/dp=3, the only possible arrangement for spheres within a cylinder (or for discs within a larger circle) is one sphere at the center with six spheres tangent to the tube wall. Thus, one can also intuitively argue that randomness decreases as order is imposed on the packing. Recall the experiments of Gunn and Pryce (1969); with the Fickian model, which implies randomness, they were unable to reproduce observed dispersion behavior in intentionally ordered packed beds. (In practice, such ordered cases arise in applications involving highly exothermic catalytic reactions. Usual practice is to pack only a few pellets across the tube diameter so that effective cooling can be achieved and hot spots, particularly at the tube axis, can be avoided.)

Model Development

If a cylindrical tube is packed with inert uniformly sized spheres, the simplest mass dispersion cases are the steady-state injection of dye, or tracer, on the tube axis and a transient step-change in concentration across the entire inlet cross-section. For these cases, two AFM parameters define the dispersion behavior: the number (size) and distribution of radial plugs within each A or B half-cell and the length of each repeating A/B cell (see Figure 2). The distribution of the flow among the individual radial plugs, or the split-merge behavior, follows from these dimensions via a hydraulic resistance argument.

Consider as an example a tube divided into six concentric annuli as shown in Figure 2. Since the flow into a channel or arbitrary cross-section is described by

$$\Delta P = f\left(\frac{L}{Rh}\right) U^2/2g_c \tag{2}$$

and

$$f = \begin{cases} \text{constant/Re} & \text{laminar} \\ \text{constant} & \text{turbulent} \end{cases} \tag{3}$$

the total flow, Qt, entering a pipe of pattern A (Figure 2) will be distributed to each plug as

$$Q_i/Qt = (1/H_i)\Sigma(1/H_i) \quad i=2,4,6 \tag{4}$$

In the above relationship, the individual hydraulic resistances Hi, depend on annulus dimensions and on flow regime (Appendix B) as

$$1/Hi = \begin{cases} A_i Rh_i^2 & \text{laminar} \\ A_i (Rh_i)^{0.5} & \text{turbulent} \end{cases} \qquad (5)$$

Here, whether the flow be regarded as laminar or turbulent is based on the particle Reynolds number, Re_p (pellet diameter as characteristic length) for flow around individual spheres; $Re_p > 150$ implies turbulence, and $Re_p < 150$ implies laminar flow. As the fluid flows from the A-half-cell to the B-half-cell, the plug 2 flow splits in proportion to the hydraulic resistances presented by plugs 1 and 3, the plug 4 flow splits in proportion to the plug 3 and 5 resistances, and the plug 6 flow must all enter plug 5 (Figure 2), i.e.,

$$\begin{aligned} Q_1/Qt &= (1-W_3)Q_2/Qt \\ Q_3/Qt &= W_3 Q_2/Qt + (1-W_5)Q_4/Qt \\ Q_5/Qt &= W_5 Q_4/Qt + Q_6/Q_t \end{aligned} \qquad (6)$$

The individual weighing factors are determined by the resistances of those B plugs into which each A plug must split. Consider, for example, A-plug 4 as it splits via two competing resistances into B-plugs 3 and 5 (just as there were three competing resistances for the total flow entering pattern A). Thus

$$Q_5/Q_4 = \frac{1/H_5}{1/H_5 + 1/H_3} = W_5$$

and (7)

$$Q_3/Q_4 = \frac{1/H_3}{1/H_3 + 1/H_5} = 1-W_5$$

Hence, the weighing factors of equation (6) are given by

$$W_i = \frac{1/H_i}{1/H_i + 1/H_{i-2}} \tag{8}$$

where the subscripts are as illustrated in Figure 2 and the hydraulic resistances are as defined in equation (5), above. As the fluid moves from the B-half-cell into the next A-half-cell, the plugs recombine in such a way as to regain the original A distribution. This implies that the concentration entering each plug is a weighed average of the outlets of preceding plugs:

A to B transition

$$C_1 = C_2$$

$$C_3 = (1-W_5)Q_4C_4 + W_3Q_2C_2 \,/Q_3$$

$$C_5 = W_5Q_4C_4 + C_6Q_6 \,/Q_5$$

B to A transition (9)

$$C_2 = W_3C_3 + (1-W_3)C_1$$

$$C_4 = (1-W_5)C_4 + W_5C_3$$

$$C_6 = C_5$$

(Note: the question may arise as to why the AFM employs the A-first pattern as opposed to the B-first pattern. Since the profiles predicted by the AFM are insensitive to the A/B order (Figure 3, Table 2) the A-first pattern was selected.)

Table 2

Centerline Concentrations for two AFM Patterns

Dt/dp	z/dp	C/Ca at r=0 A-B	B-A
25.6	52	8.6	8.2
13.3	27	4.2	4.1
11.1	23	4.0	3.7
6.9	14	2.2	2.4
19.2	52	4.8	5.0
8.3	23	2.0	2.3
12.8	52	2.1	2.1
5.3	23	1.3	1.3

These geometries correspond to data taken by Fahien and Smith (1955). Model is compared to data in a later section.

For the simple mass dispersion only cases, the plug flow equation for each radial plug becomes

$$u\, dC/dz + dC/dt = 0 \qquad (10)$$

where determination of the individual linear velocities, u, are discussed below. The solution of equation (10) indicates that the concentration at the outlet of each radial plug is simply its input signal delayed by a dead time equal to the half-cell length divided by u. Since the fluid must traverse a series of delays before exiting the bed, a finite time will pass before any inlet changes will propagate to the outlet.

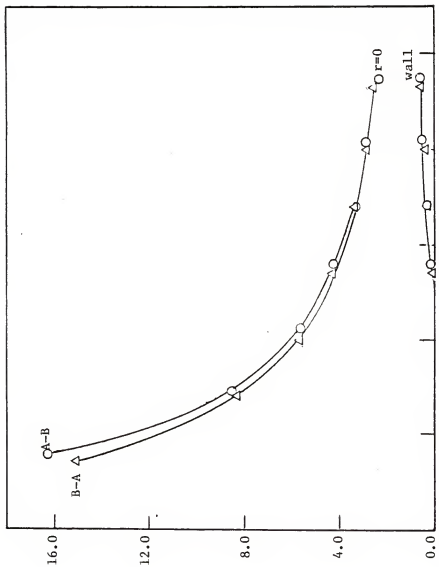


Figure 3: A-first and B-first APM Concentration Profiles

In the steady-state, enough time has passed so the outlet and inlet concentrations are equal and the concentration profile at the n-th axial segment can be determined from the inlet profile:

$$\underline{A}_n = (\underline{\underline{S}}\underline{\underline{R}})^{n-1}\underline{C}_{in} \qquad (11\text{-a})$$

$$\underline{B}_n = \underline{\underline{R}}\underline{A}_n$$

where

$$\underline{A}_n^T = [C_{2,n}\ C_{4,n}\ \cdots\ C_{Nrad,n}]$$

$$\underline{B}_n^T = [C_{1,n}\ C_{3,n}\ \cdots\ C_{Nrad-1,n}] \qquad (11\text{-b})$$

$$\underline{C}_{in}^T = [C_{2,in}\ C_{4,in}\ \cdots\ C_{Nrad,in}]$$

and $\underline{\underline{R}}$ and $\underline{\underline{S}}$ are each (Nrad/2) by (Nrad/2) di-diagonal matrices with all elements zero except that

$$s_{i,i} = \begin{cases} 1-W_{2i} & i=1,2,3,\ \ldots,(Nrad/2) \\ 0 & i=Nrad/2 \end{cases}$$

$$s_{i,i+1} = \begin{cases} W_{2i} & i=1,2,3,\ \ldots,(Nrad/2) \\ 1 & i=Nrad/2 \end{cases} \qquad (11\text{-c})$$

$$r_{i,i} = \begin{cases} 1 & i=1 \\ \dfrac{W_{2i-2}Q_{2i-2}}{Q_{2i-1}} & i=2,3,4,\ \ldots,\ (Nrad/2) \end{cases}$$

$$r_{i,i+1} = \begin{cases} 0 & i=1 \\ \dfrac{(1-W_{2i})Q_{2i}}{Q_{2i-1}} & i=2,3,4,\ \ldots,\ (Nrad/2) \end{cases}$$

Here, Nrad signifies the total number of void radial plugs in an A/B cell. Note that a point source of dye is simulated by setting $C_{2,in}$ = Cin and $C_{4,in} = C_{6,in} = \ldots = C_{Nrad,in} = 0$. Since the concentration in any given radial plug is solely a function of upstream conditions, no backmixing is predicted.

In the transient case, the dead times are most easily viewed in the Laplace domain. A uniform step-change in inlet concentration is simulated by setting all elements of an (Nrad/2)-long column vector equal to (Cin/s). The concentration profile at the nth axial segment and at any given time can be represented in a form analogous to equation (11), above, with additional inclusion of diagonal delay matrices:

$$\begin{aligned} \underline{A}_{out,n} &= \underline{\underline{\theta}}_A \underline{A}_{in,n} \\ \underline{B}_{out,n} &= \underline{\underline{\theta}}_B \underline{B}_{in,n} \end{aligned} \qquad (12\text{-a})$$

where $\underline{\underline{\theta}}_A$ and $\underline{\underline{\theta}}_B$ are diagonal matrices with elements

$$\begin{aligned} (\theta_A)_{i,i} &= \exp(-sd_j) \qquad i=1,2,3,\ \ldots,\ Nrad/2 \\ & \qquad\qquad\quad j=2i \\ (\theta_B)_{i,i} &= \exp(-sd_j) \qquad i=1,2,3,\ \ldots,\ Nrad/2 \\ & \qquad\qquad\quad j=2i-1 \end{aligned} \qquad (12\text{-b})$$

so that

$$(\underline{A}_{in})_n = (\underline{\underline{S}}\underline{\underline{\theta}}_B \underline{\underline{R}} \underline{\underline{\theta}}_A)^{n-1} \underline{C}_{in}/s$$

$$(\underline{B}_{out})_n = \underline{\underline{\theta}}_B \underline{\underline{R}} \underline{\underline{\theta}}_A (\underline{\underline{S}}\underline{\underline{\theta}}_B \underline{\underline{R}} \underline{\underline{\theta}}_A)^{n-1} \underline{C}_{in}/s$$

Note that equation (12) implies a radial distribution of the total time delay required for an inlet change to be seen at the outlet, i.e., a residence time distribution. The matrix formulation of equation (12) is for convenience. The actual mechanics of real-time simulation are described in Appendix E.

Now that the appropriate describing equations have been established, the corresponding radial plug size distribution axial cell length and individual linear velocities must be determined.

Alternating Flow Model Parameters

As mentioned earlier, radial variations in bed voidage, as porosity, are well-documented experimentally (see Appendix C) and have been correlated via a tri-regional model (Cohen and Metzner, 1981) which is shown below for convenience:

1. wall region ($x<0.25$)--

$$1-\varepsilon = 4.5(1-\varepsilon_b)(x-7x^2/9)$$

2. transition region ($0.25<x<8$)--

$$\frac{\varepsilon-\varepsilon_b}{1-\varepsilon_b} = a_1 e^{-a_2 x}\cos(a_3 x - a_4)\pi \qquad (13)$$

3. bulk region ($x>8$)--

$$\varepsilon=\varepsilon_b$$

where x is the distance, in pellet diameters, from the tube wall; the constants are a_1=0.3463, a_2=0.4273, a_3=2.4509, a_4=2.2011. It should be noted that these radial porosities are averaged over the entire bed length.

Although the literature only hints at axial voidage variations (Bennett, 1972; Schwartz and Smith, 1953), they do exist. Consider again the case of dropping spheres into a vertical cylinder whose diameter is three times that of an individual sphere. The densest packing is to have repeating layers of seven spheres (one in the center and six tangent to the wall), with the outside ring of spheres rotated thirty degrees from the layer below and the center spheres stacked one on top of the other. The area void fraction will be maximum, i.e.,completely empty, at the tube bottom and will decrease to a minimum at one-half pellet diameter up. The void fraction will again increase (to a different maximum) as one moves halfway to the center plane of the next layer and then decrease (to a different minimum) at the center plane, and so on. One can also extend this idea of repeating axial layers to more complex packing arrangements, i.e., larger Dt/dp. Figure 5 shows numerically determined axial void variations for Dt/dp=3 whereas Figure 4 shows experimentally measured voidages Dt/dp=6.6. The numerical and experimental techniques are described in Appendix D.

The peak-to-peak distance in the void fraction curves indicates the number of void-full regions expected both radially and axially.

Radially, this distance can be found by determining the points at which $\varepsilon=\varepsilon_b$ (equation (13)) and are

$$\cos(a_3 x - a_4)\pi = 0$$

or

$$a_3 x - a_4 = \ldots -3/2,\ -1/2,\ 1/2,\ 3/2,\ \ldots, \qquad (14)$$

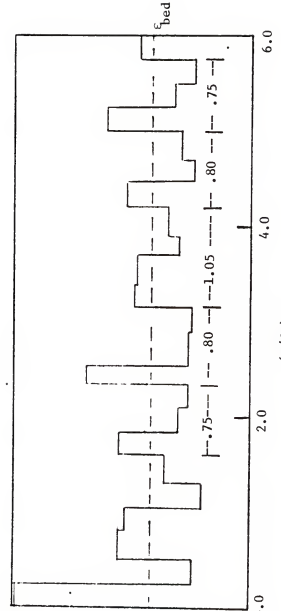


Figure 4: Axial Voidage Variations, Dt/dp=5.04, Measured Experimentally

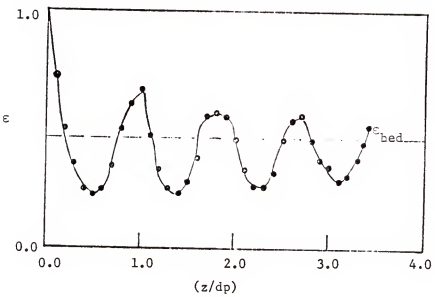


Figure 5: Axial Voidage Variation, Dt/dp=3.0, Determined Numerically

The radial thickness of each void-full region would then be the distance between the i-th and (i+2)th zeros, since each zero indicates a transition from maximum to minimum voidage. Note from Table 3 the distance between successive zeros is 0.408 dp, yielding a radial void-full thickness of 0.816dp. (It may be of interest to also note that the center-to-center distance between spheres arranged in a hexagonal close packed (HCP) pattern is 0.816dp). Thus, Nrad=(Dt/dp)/0.816, to the next highest even integer, and the radius is divided into (Nrad/2) equal increments which are then subdivided to satisfy the radial distribution of void fraction. That is, the voidage of any given A- or B-plug must equal the radially averaged voidage given by equation (13) for that same interval:

$$2\int_{r_i}^{r_{i+2}} r\,\varepsilon(r)\,dr = r_{hi}^2 - r_{lo}^2 \qquad (15)$$

where the small r's denote the scaled radial position, R/Rtube. The radii r_{hi} and r_{lo} are determined by the half-cell as shown in Figure 6. (Note that for the A-half-cell r_{lo} is unknown, hwereas for the B-half-cell r_{hi} is unknown). The corresponding overall bed voidage ε_{bed} can be found by integrating the left hand side of equation (15) from r=0 to r=1 and is not necessarily equal to ε_b of equation (13). Thus, ε_b must be selected to give ε_{bed} within a few percent of the observed value. If the overall bed voidage is unknown, the comprehensive data of Leva and Grummer (1947b) for bed voidage as a function of Dt/dp can be used.

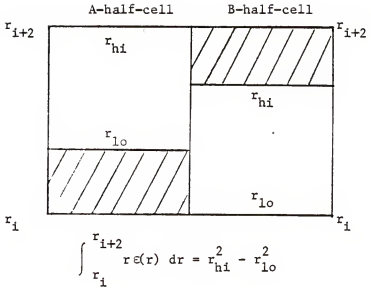


Figure 6: Intermediate Radius Integration Limits

Table 3

Half-cycle Crossings of Radial Void Function

R.H.S. of equation (14)	x-value
-1.5	0.286
-0.5	0.694
0.5	1.102
1.5	1.510
2.5	1.918
3.5	2.326
4.5	2.734

Axially, the peak-to-peak distance can be found in an analogous manner. Figures 5 and 4 show the cycle width, which represents the length of one half-cell, to be approximately 0.82dp, independent of Dt/dp. Recall that the center-to-center distance for HCP spheres is 0.816dp; it is therefore assumed that this is the axial voidage cycle width. Thus, the total (A/B) cell length is twice that amount giving Nz=Ztot/1.632dp as the number of repeating (A/B) cells.

The individual linear velocities, u (equation (10)), are calculated as volumetric flow rate (equations (4) and (6)) divided by cross-sectional area of flow, $u_i = Q_i/A_i$, as was implied by employing equation (2) to distribute the flows. The individual cross-sectional areas, A_i, are determined from the radii defined by equation (15). These velocities are scaled by dividing the average interstitial bed velocity, $u = Qt/\varepsilon_{bed}Atube$, or

$$u_i/u' = \frac{\varepsilon_{bed}(Q_i/Q_t)}{A_i/Atube}$$

The delay times in each annulus are given by the plug (or half-cell) length divided by the corresponding velocity and are scaled by dividing by the average bed hold-up time, τ = Ztot/u , to give

$$d_i/\tau = \frac{A_i/Atube}{2Nz\ \varepsilon_{bed}\ Q_i/Qt} \qquad (17)$$

since there are (2 Nz) half-cells (plug lengths) across the overall bed length, Ztot.

Figures 7 - 12 compare observed radial profiles of u_i/u' to those predicted by equation (16). In all cases, the AFM predictions follow the data well. In these figures, the AFM profiles are represented by horizontal bars corresponding to the A- or B-plugs (B with hash-marks, A without); the non-vertical dashed segments connect across those regions the AFM considers occupied by solid regardless of half-cell (refer to Figure 2). The experimental data are represented in Figures 8 - 12 by horizontal bars covering the regions in which the respective researchers assumed the velocities to be constant. In these cases, velocities were measured at five radial positions each with 10% of the total tube cross-sectional area on either side so that the radially integrated (average) velocity, u', would equal the arithmetic average. In Figure 7, the data are represented by single points since so many measurements were made. In this case, the radially averaged velocity, u', was determined by numerical integration from which the scaled values were calculated.

Because insertion of velocity probes into the packing would disrupt both the flow profile and packing arrangement, velocity data were taken in the empty tube some distance beyond the packed section. As this distance increases, the velocity profile tends to flatten out (Figure 13) and eventually approaches the roughly parabolic shape expected in an empty tube. In addition, velocities will decrease when the fluid expands from the small cross-section

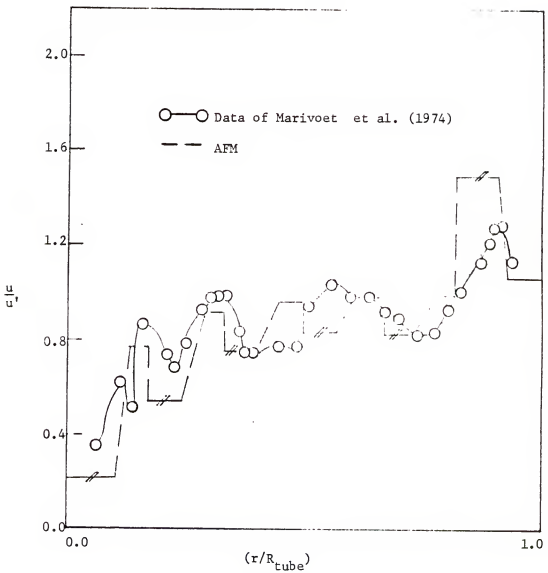


Figure 7: Radial Velocity Profiles, Dt/dp=9.4, 3" Pipe, Data (Marivoet et al., 1974) Taken 0.5cm beyond Packed Section

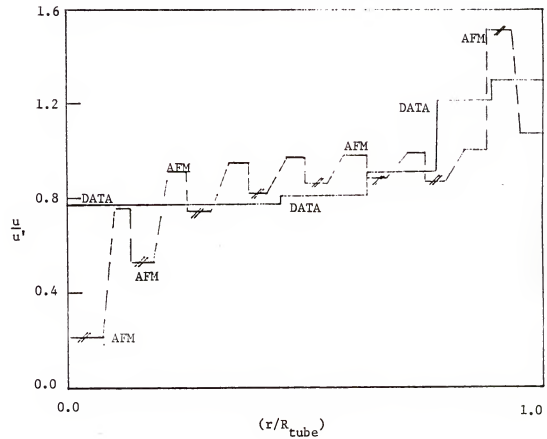


Figure 8: Radial Velocity Profiles, Dt/dp=]3.2, 4" Pipe, Data (Schertz and Bischoff, 1969) Taken 1 inch beyond Packed Section

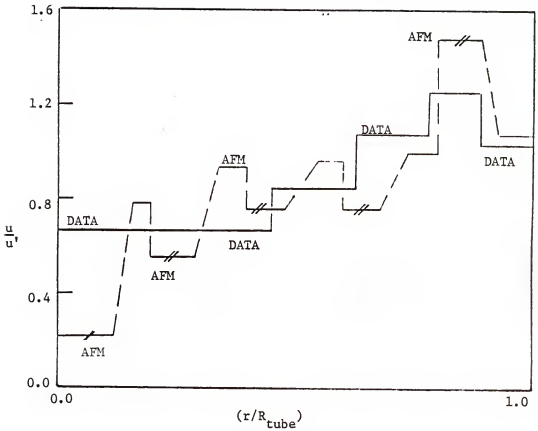


Figure 9: Radial Velocity Profiles, Dt/dp=8, 4" Pipe, Data (Schwartz and Smith, 1953) Taken 2 inches beyond Packed Section

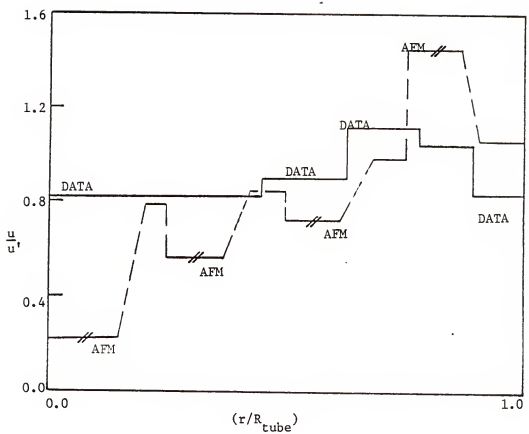


Figure 10: Radial Velocity Profiles, Dt/dp=6, 3" Pipe, Data (Schwartz and Smith, 1953) Taken 2 inches beyond Packed Section

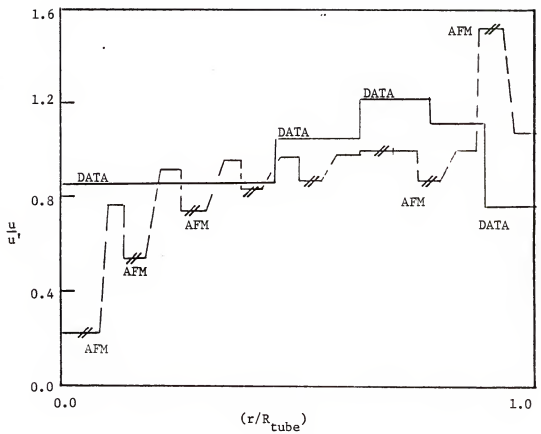


Figure 11: Radial Velocity Profiles, Dt/dp=12.8, 2" Pipe, Data (Schwartz and Smith, 1953) Taken 2 inches beyond Packed Section

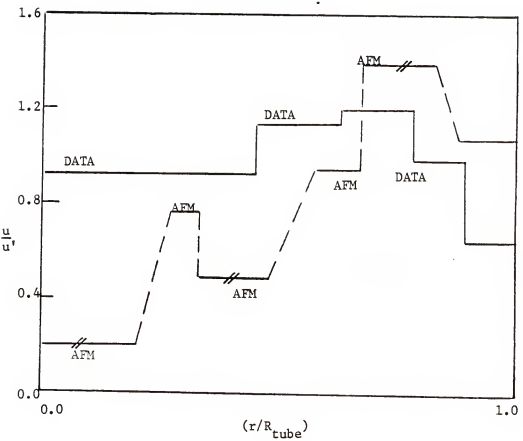


Figure 12: Radial Velocity Profiles, Dt/dp=5.3, 2" Pipe, Data (Schwartz and Smith, 1953) Taken 2 inches beyond Packed Section

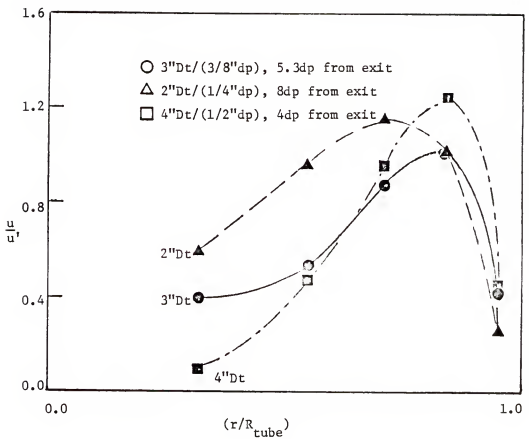


Figure 13: Flattening of Radial Velocity Profile as Distance beyond Packed Section Increases, Dt/dp=8, Data (Schwartz and Smith, 1953) Taken 2 inches beyond Packed Section, Regardless of Dt

of the packing interstices into the larger cross-section of the empty tube. The degree of expansion probably varies radially due to the radial porosity profile with the smallest effect at maximum voidage near the wall. But, the empty tube wall drag and tendency for maximum velocity at the centerline would likely combine to dampen out any peaks near the wall more dramatically than at other radial positions. Vortmeyer and Winter (1982) solved the Navier-Stokes equations for an empty tube with a maximum-near-wall velocity profiles at its inlet and showed that the flow pattern quickly redistributes. However, the empty tube measurements should at least indicate the velocity trends within the packing.

In all cases, the AFM predictions follow the observed velocity trends. Moreover, the AFM predictions more closely match data taken either very close to the bed exit (Figure 7) or in larger tubes (Figure 8 and 9) where the empty tube has had less of a chance to influence the flow patterns. This good agreement of predicted and measured velocities gives credibility to using equations (16) and (17) to determine transient characteristics of packed beds.

Examination of these techniques for determining AFM parameters reveals one key point: only geometric factors (Dt/dp, z/dp, ϵ_{bed}) are required to predict mass dispersion in packed beds. Thus the Alternating Flow model is predictive; its parameters are determined a priori with no need for back-fitting them to dispersion data. In a later section, steady-state data will be used to check the sizing of axial cell length, the distribution of radial plugs, and the

distribution of flows. Transient data will be used to check the velocity (delay time) distribution. But first, some limitations of the AFM must be discussed.

Model Limitations

Questions regarding how the Alternating Flow model handles the cases of

1. zero bulk velocity or flow rate,
2. extremely wide beds (i.e., Dt/dp large),
3. extremely long beds (i.e., z/dp large)

may arise. Each is discussed below.

Zero velocity dispersion behavior should reduce to a pure diffusion-like mechanism. Consider the simplest steady-state experiment of injecting dye (tracer) at some point within the packed bed. If there is no bulk velocity, then the dye should disperse equally in both directions; that is, there must be back-mixing. A model, such as the AFM, which alleviates the back-mixing problem described earlier, cannot describe such zero velocity behavior. But, any model, such as the Fickian analogy, which can describe stagnant flow fails to alleviate the back-mixing problem.

For the AFM, extremely wide or long beds result in large numbers of radial plugs or axial cells, respectively. As these numbers become increasingly large, the AFM description of the transient (F-curve) behavior approaches plug flow behavior for the overall bed, i.e., the output signal becomes the input signal delayed by one bed hold-up time. This is a result of flat radial delay-time profiles (equation (17)). As Dt/dp increases, the "wall region" becomes a

smaller proportion of the total bed cross-section thus creating a more uniform porosity profile, which in turn implies more uniform velocity and delay time profiles. As z/dp increases, Nz follows and the denominator of equation (17) eventually becomes large enough to prevent any noticable differences between individual delay-times.

Comparison with Experimental Data

Figures 14 - 17 give steady-state radial concentration profiles at a set of positions for $5.6<Dt/dp<54$, $100<Re_p<500$, and 10 z/dp 100. Figure 18 shows axial profiles at two set radial positions for Dt/dp=12.8, and Figures 19 and 20 give F-curves for Dt/dp=15.9 and 8.0. Both gases and liquids are represented (Table 4). Experiment is compared to prediction via

1. Fickian predictive: dispersion coefficients obtained via correlations available in the literature (Wen and Fan, 1975; Levenspiel, 1962;
   a) steady-state via equation (15) of Gunn and Pryce (1969),
   b) transient via equation (19) of Danckwerts (1953),
2. Alternating Flow Model predictions.

These figures do not show profiles obtained by back-fitting dispersion coefficients to the data since, at any given axial position, it is possible to obtain a nearly perfect fit. However, as indicated by the experiments of Fahien and Smith (1955) these coefficients may change with axial position.

Table 4

Data Used for Mass Dispersion Comparison

Source	Type[a]	Dt	dp	Tracer/ bulk	Rep	z/dp
Fahien and Smith (1955)	SS	2"-4"	5/32" -0.36"	CO_2/air	150 -900	10-70
Gunn and Pryce (1969)	SS	3.5"	6mm	Ar/air	121	23
Latinen (1951)	SS	2"	.037"	dye/water	102	180
Cairns and Prausnitz (1960)	trans	2"	3.2mm	NaCH/water water	128	191
Jacques and Vermeulen (1957)	trans	6"	.75"	NaCH/ water	130[b]	32

[a] SS=steady-state; trans=transient.

[b] Data read directly from their Figure 32, which was assumed to represent Run 217-2 (2gpm) and not Run 217-1 as stated. If this assumption is not made, the data imply that the F-curve reaches 50% only after two vessel hold-up times, a situation that seems highly unlikely.

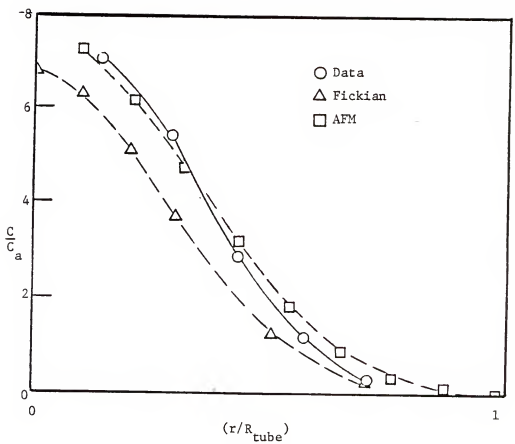


Figure 14: Steady-state Radial Concentration Profiles, Dt/dp=15, Z_{tot}/dp=23, Data of Gunn and Pryce (1969)

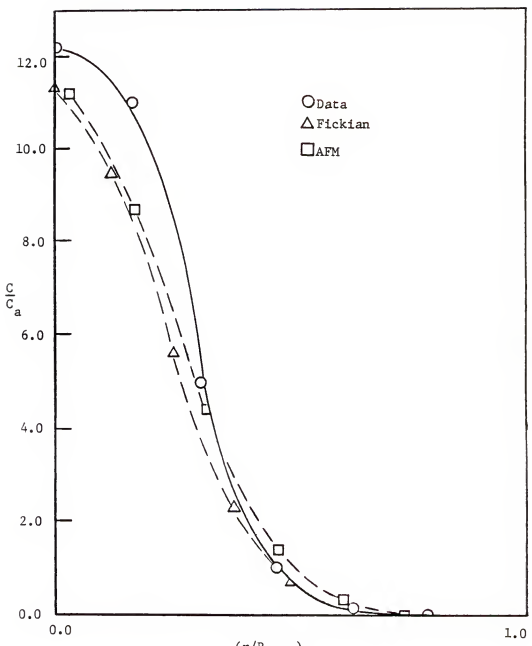


Figure 15: Steady-state Radial Concentration Profiles, Dt/dp=54.3, Z_{tot}/dp=180, Data of Latinen (1954)

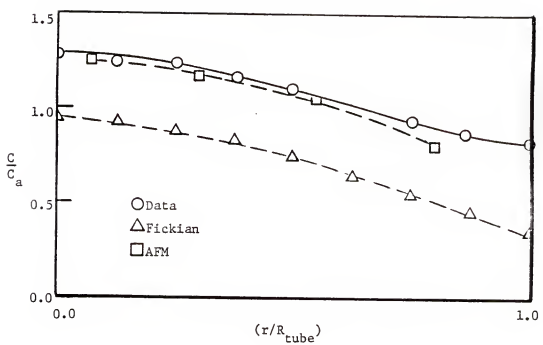


Figure 16: Steady-state Radial Concentration Profiles, Dt/dp=5.6, Z_{tot}/dp=23, Data of Fahien and Smith (1955)

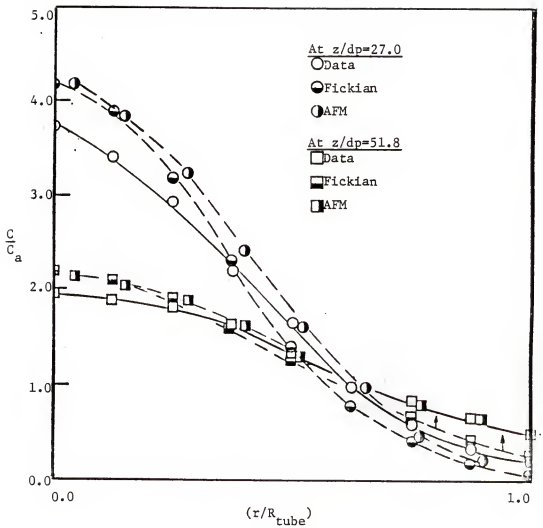


Figure 17: Axial Variation of Steady-state Radial Concentration Profiles, Dt/dp=12.8, z/dp=27 and 52, Data of Fahien and Smith (1955)

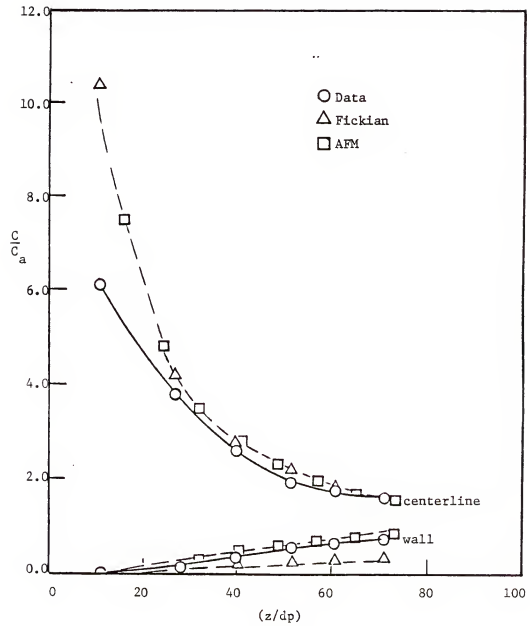


Figure 18: Steady-state Axial Concentration Profiles, Dt/dp=12.8, Data of Fahien and Smith (1955)

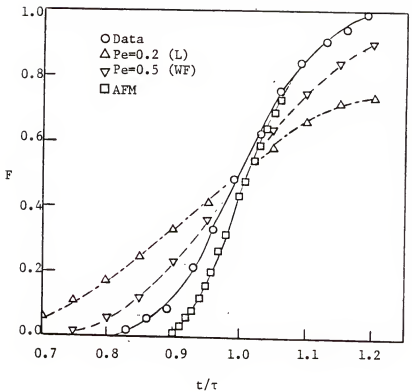


Figure 19: F-curves for Dt/dp=15.9, Z_{tot}/dp=191, Data of Cairns and Prausnitz(1960), L=Levenspiel (1962), WF=Wen and Fan (1975)

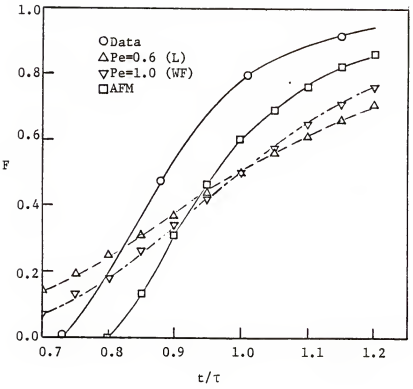


Figure 20: F-curves for Dt/dp=8.0, Z_{col}/dp=32, Data of Jacques and Vermeulen (1957), L=Levenspiel (1962), WF=Wen and Fan (1975)

In the steady-state Figures (14 - 18), the vertical axis represents point-value concentrations scaled by the average measured effluent concentration, Ca, which can be calculated at any given axial position as Ca = (total amount of tracer material)/(total amount of fluid). Solutions of the Fickian analogy (equation (1)) for C/Ca as function of radial and axial position are given elsewhere (e.g., Roemer et al., 1962; Gunn and Pryce, 1969; Danckwerts, 1953; Cairns and Prausnitz, 1960; Wen and Fan, 1975). For the AFM the scaled concentrations become

$$C_i/Ca = C_i Q_i / \Sigma(Q_j C_j) \qquad (18)$$

with j=2,4,. . .,N for the A-half-cell, and j=1,3,. . .,N-1 for the B-half-cell. The subscript "i" implies that the concentration in that given annular plug is constant. To alleviate discrete (stepwise) concentration profiles, Figures 14 - 18 show the values calculated from equation (18) at each plug's midpoint radius.

Figures 14 - 16 indicate good agreement of the AFM with experiment over a wide range of Dt/dp. However, Figures 17 and 18 which show axial variations for Dt/dp=12.8 indicate that, at low z/dp, neither the AFM nor the Fickian analogy closely follows the observed dispersion behavior. However, the agreement is quite good at z/dp>25.6 or two tube diameters. This behavior is also borne out in Table 5 which compares AFM and Fickian predictions to observed values of centerline concentrations for 5.6<Dt/dp<25.6 as given by Fahien and Smith (1955). Note the improvement in both models as z/Dt increases. This can probably be attributed to entrance effects

since the tracer injection tube creates a disturbance in the flow pattern and in the packing pattern which may each take some distance to settle out. For example, in empty tubes the flow disturbance created by a barrier requires several pipe diameters to settle out (Daugherty and Franzini, 1977) as compared to an apparent "settling length" here of about two pipe diameters. This shorter distance should be expected since the packing tends to impose order on the flow pattern. Consider also that insertion of a tracer injection tube into the packing will disrupt the "normal" packing arrangement and hence the distribution of voids. Thus, the assumed plug and cell distributions may not be applicable in the vicinity of the injection tube. In fact, Marivoet et al. (1974) showed that insertion of a narrow tube along the axis of a packed bed significantly altered the flow pattern.

Given such arguments, one would expect this entrance effect to disappear if there is no physical barrier inserted into the packing. Since the simplest heat-dispersion-only experiments meet the no-barrier criterion, the corresponding AFM results should provide more insight into this entrance effect.

In all steady-state cases, the AFM results equal or surpass the Fickian predictions. These results lend support to the previously described techniques for sizing plugs (equation (15)), for determining cell length (HCP spacing) and for distributing the flows (equations (6) and (7)).

Table 5

Centerline Concentrations--Data, Fickian, and AFM

Dt/dp	z/dp	z/Dt	Centerline Concentration[a]		
			Data	AFM	Fickian
25.6	52.0	2.0	4.8	8.6	8.7
13.3	27.1	"	2.8	4.2	4.5
11.1	22.6	"	2.3	4.0	3.7
6.9	14.0	"	1.3	2.2	2.3
19.2	52.0	3.0	3.8	4.8	4.9
8.3	22.6	"	1.8	2.0	2.1
12.8	52.0	4.0	2.2	2.1	2.2
5.6	22.6	"	1.3	1.3	.95

[a]All data from Fahien and Smith (1955).

Transient (F-curve) AFM and Fickian predictions using dispersion coefficients from two different sources (Levenspiel, 1962, p. 282; Wen and Fan, 1975, p. 166) are compared to data in Figures 19 and 20 (see Table 4 for system description). These figures indicate that the Alternating Flow model again surpasses the Fickian analogy, even in the case of the longer bed (Figure 19, z/dp=191). In this case, the AFM might be expected to fail because of its tendency to predict plug flow behavior for the overall bed for large z/dp and Dt/dp as noted in the "model limitations" discussion, above.

The log of the AFM behind the data may be due to using an incorrect ε_{bed} in determining velocity profiles. The ε_{bed} value used in the AFM simulations for Figures 19 and 20 were based on the ε_{bed} versus Dt/dp data given by Leva and Grummer (1947b) since neither researcher gave explicit bed porosity values. If ε_{bed} is actually larger than the selected values, then the scaled velocities would be proportionately faster and the entire AFM F-curve would shift left in time. The shift should become less pronounced as the number of mixes increases since increasing the exponent (axial cell number, n) or dimension (Dt/dp or Nrad) of equation 11 tends to dampen any discontinuities in the velocity profile. Comparisons of Figures 19 and 20 supports this reasoning since the lag appears constant for the shorter, narrower bed (Figure 20) but approaches zero for the longer, wider bed (Figure 19). The steady-state results are more tolerant of ε_b errors: ε_b was estimated (from the data of Leva and Grummer, 1947) for some of the cases and AFM predictions still closely

followed the concentration data. This can be attributed to the fact that the number and thickness (or hydraulic radius) of radial plugs determine steady-state mixing characteristics. Recall the assumption that the radial porosity profile will oscillate with the same frequency regardless of its mean value. Thus, the effect of ε_b on Nrad is nil and on the radial plug thicknesses is minimal.

CHAPTER III
HEAT DISPERSION

Consider now the heating of a gas, initially at uniform temperature, Tin, as it flows through a packed bed with constant wall temperature, Twall (Figure 21). Heat transfers in from the wall so that radial temperature gradients will be the sharpest just inside the bed and will flatten with increasing axial position. If the bed is long enough, the fluid will eventually reach a uniform temperature of Twall.

The corresponding Fickian analogy assumes that heat flows in at the wall by a film resistance and then disperses radially by conduction through a pseudo-homogeneous medium, or (in the steady-state)

$$u \frac{\partial T}{\partial z} - \lambda \frac{\partial^2 T}{\partial z^2} - \lambda \frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r}\right) = 0 \qquad (19)$$

where λ = effective thermal conductivity of the packed section ("effective" to account for void fraction), $G=\rho$ G/Atube is the mass flux, ρ is the fluid density, and Atube and G are defined earlier. The well-known solution of equation (19) with appropriate boundary conditions and the usual assumption of no axial dispersion is a Bessel function series (e.g., Li and Finlayson, 1977). The boundary conditions give rise to a wall film heat transfer coefficient, hw. The parameters, hw and λ, are either fit to experimental data or

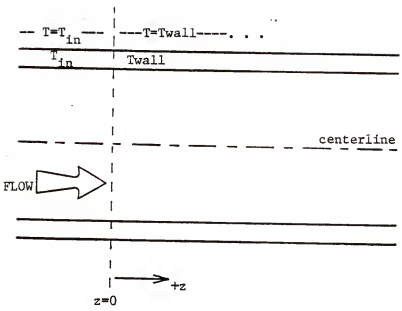


Figure 21: Simplest Heat Dispersion Experiment

obtained from available correlations giving these coefficients in dimensionless form in terms of Re_p (see Appendix G for list of references). However, experimental values of hw depend on axial position and corresponding λ depend on both axial and radial position (Bunnel et al., 1949; Calderbank and Pogorski, 1957; Coberly and Marshall, 1951; deWasch and Froment, 1972; Hall and Smith, 1949; Kunii et al., 1968; Kwong and Smith, 1957; Lerou and Froment, 1977; Li and Finlayson, 1977; Patterson and Carberry, 1983; Plautz and Johnstone, 1955) so that average or asymptotic values must be used. The literature provides many forms of correlations for both hw and λ (e.g., Carberry, 1976; Froment and Bischoff, 1979; Li and Finlayson, 1977; Schlunder, 1978). The "data effect" may cause the "correlation effect" but both may be due to several factors:

1. assumption of radially uniform velocity in equation (19)
2. assumption of radially uniform λ in equation (19)
3. misrepresentation of the Reynolds number (correlation effect only)
4. erroneous application of the Fickian analogy.

Schlunder (1978) points out that using a non-uniform velocity profile decreases the dependency of hw on tube length.

The first two points were also considered by Lerou and Froment (1977) who included a prescribed radial profile in G (i.e., velocity) and a given functional form for λ versus Re (local) in fitting point values of $\lambda(r)$ and overall values of hw to their experimental data. They reasoned that because there are both static and turbulent con-

tributions to λ it must vary radially for two reasons: the porosity profile (static contribution) and the velocity profile (turbulent contribution). To support this reasoning they fit the parameters to the model with uniform λ to the model with point values of $\lambda(r)$. In both models they obtained better fits by allowing G to vary inversely with porosity, in contrast to the observed velocity profiles which were discussed earlier. Although no direct comparison was made between data and temperature profiles predicted by the uniform and point-value models, it was implied that the latter gave better results. However, in over two thirds of the experiments listed, application of the point-value λ model increased the uncertainty in the absolute value of hw; the relative uncertainty increased in about half of the cases.

Hence, allowing λ to vary radially can improve temperature profile predictions but may decrease the confidence with which hw can be regarded. Note also that it was necessary to employ erroneous velocity profiles to attain these results. Thus the added accuracy may be due to increasing the number of parameters (allowing λ to vary radially) and not due to better representation of the Fickian parameter.

Next, consider the correlation of λ and hw in terms of Re_p. As discussed earlier, the particle Reynolds number may not be the best descriptor of turbulence in packed beds. Some attempt has been made to use other "hydraulic" Reynolds number (Li and Finlayson, 1977), but these have remained relatively unpopular.

And next consider application of the Fickian model to dispersion in packed beds. If the model is truly applicable, then the observed spatial variations in its parameters should be justified. Because the usual practice is to neglect axial heat conduction in the Fickian analogy (equation (19)) the literature provides little information for non-stagnant effective axial thermal conductivities especially in cases where simultaneous axial and radial conduction is considered (Clement and Jorgensen, 1981; Patterson and Carberry, 1983; Wakao, 1976; Wakao et al., 1979; Yagi et al., 1960). But, under the assumption of pseudo-homogeneity implied by equation (19) a total absence of axial heat "conduction" seems unlikely. Thus, spatial variations in radial thermal conductivity may be needed to compensate for otherwise ignored driving forces in the axial direction. The radial variation of conductivity can also be justified on porosity variations since the relative ratio of solid to fluid will change accordingly. But what about the axial variation in hw? In empty tubes, hw will vary from some high value in the entrance region (because of increased turbulence there) and will eventually settle out to some constant value (e.g. McCabe and Smith, 1976). Thus, length-averaged hw's for empty tubes depend on total tube length. Packed beds, however, have no single entrance region after which the turbulence settles out. They are, in fact, a large number of entrance regions in series since the fluid moves through repeating layers of pellets. Because each entrance region, or layer, is short

(less than one pellet diameter) one would expect hw to be constant throughout the length of the bed.

Furthermore, as the mass dispersion chapter points out, the Fickian analogy implies random fluid motion whereas flow through packed beds is orderly. Although heat transfers by many mechanisms (conduction, turbulent and film convection, radiation) which may or may not be orderly, recall the simplicity of the heat dispersion being described. Heat transfers in from the wall at a temperature low enough to rule out radiation, through a film to a gas of low thermal conductivity. The gas moves around packing made from a material (e.g., glass or catalyst support) again of low thermal conductivity. Any heat transferred to the packing must pass through a film, and the amount of heat transferred is small. Thus, the overriding mechanism is convection--through films and by bulk fluid motion.

The acceptability criteria for a packed bed heat dispersion follow those presented earlier for mass dispersion. Heat must be conserved and travel at a finite speed, heat should disperse both radially and axially, and no backmixing should be predicted. The model should also properly represent the flow around packing, its solution should be straightforward and its corresponding parameters should be well-defined. The finite wavefront speed and no back-mixing criteria are based on physical arguments: the inherent non-homogeneity of the packed bed induces a high resistance to heat transfer by pure conduction (consider the small contact area between

pellets); heat must therefore travel near the speed of fluid flow and should not move backwards against the direction of bulk flow. As indicated in Table 1 (mass dispersion chapter), none of the currently available models meets all criteria.

The Alternating Flow Model, therefore, combines the wall and pellets film and bulk flow mechanisms with the previously established flow patterns and mixing characteristics to describe heat dispersion in packed beds. Although the mass dispersion chapter considered spherical pellets, most reaction applications involve packing of other shapes. This chapter, therefore, addresses both spherical and cylindrical pellets. The AFM heat dispersion equations are developed and additional parameters arise, some related to packing characteristics and some related to film heat transfer. Those parameters related to packing characteristics are determined a priori, whereas the film coefficients must be based on heat transfer fundamentals. Model results are compared to experiment for both spherical and cylindrical pellets.

Model Development

The Alternating Flow Model (AFM) assumes that heat disperses axially and radially by the repeated splitting and merging of streams, in a manner analogous to the simplest cases of mass dispersion. However, in the case of heat dispersion, the packing and wall can no longer be considered inert since heat transfers in from the wall and disperses radially from the bulk fluid to the packing. In the context of the AFM, then, equations describing the solid plugs must

also be considered. Note from Figure 2 that since the radial void-full pattern depends on half-cell several types of plugs must be considered:

1. main fluid plug--an annulus surrounded by different packing annuli (e.g., plugs A2, A4, B3, and B5 of Figure 2)
2. main solid plug--an annulus surrounded by different fluid annuli (e.g., plugs A3, A5, B2 and B4 of Figure 2)
3. center solid plug--completely surrounded by same fluid plug (i.e., plug A1 of Figure 2)
4. center fluid plug--completely surrounded by same solid plug (i.e., plug B1 of Figure 2)
5. wall fluid plug--tube wall on one side and solid plug on the other (e.g., plug A6 of Figure 2)
6. well solid plug--tube wall on one side and fluid plug on the other (e.g., plug B6 of Figure 2).

The AFM assumes that no heat transfers via radiation, that no heat conducts between solid plugs, that heat convects from wall to fluid across a wall film resistance (hw) and from wall to solid across a stagnant film, and that heat convects from fluid to packing (solid plugs) across a pellet film resistance (hp). These assumptions, together with the underlying assumptions of plug flow through each of the void radial plugs and the mixing at plug outlets via the matrix mixing equations for mass dispersion, will be used to develop appropriate heat dispersion relationships for each type of plug. The resulting equations will then be expressed within the context of the

AFM. The integral nature of these equations, however, precludes condensation to matrix form. Throughout the development, lower case t refers to solid temperatures and upper case T to fluid temperatures.

Main Fluid Plug

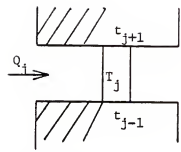
Consider a heat balance on a fluid element as shown in Figure 22-a. The element gains heat due to bulk inflow and from the warmer solid above and loses heat with the bulk outflow and to the cooler solid below. Because of the low gas thermal conductivity, this model neglects radial and axial heat conduction within the fluid itself. The heat balance thus becomes

$$\rho C_p Q_j \frac{dT_j}{dz} = hp\ a(j,j+1)\ [t_{j+1} - T_j] - hp\ a(j,j-1)[T_j - t_{j-1}] \qquad (20)$$

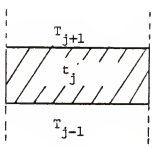
where the coordinate z refers to distance from the plug entrance, and Qj is the volumetric flow rate through the jth plug as defined for mass dispersion. Note that the mass flux G (equation (19)) is related to AFM parameters via:

$$G = \rho\ \Sigma Q_j / Atube \qquad (21)$$

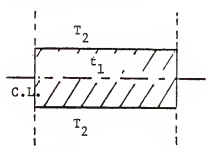
where j=2,4,. . .,N for the A-half-cell and j=1,3,. . .,(N-1) for the B-half-cell. The areas a(j.j+1) and a(j,j-1) are the areas per unit length available for heat transfer from upper solid to fluid and from fluid to lower solid, respectively. Although Figure 2 represents these areas as a single interface, their values are not simply $2\pi r$.



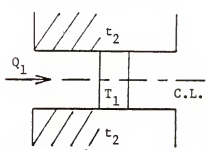
a. Main Fluid Plug



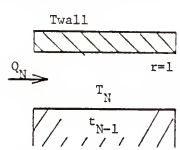
b. Main Solid Plug



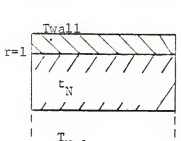
c. Center Solid Plug



d. Center Fluid Plug



e. Wall Fluid Plug



f. Wall Solid Plug

Figure 22: Plug Types for AFM Heat Dispersion Analysis

The pellet to fluid heat transfer areas are based on the total surface area available within a solid plug, i.e., the number of pellets that can fit into the solid plug volume times the surface area per pellet. It is then assumed that half of this area faces up and half down so that

$$a(j,j+1) = 0.5\pi Rtube^2(r_{j+1}^2 - r_j^2)Sp/Vp$$
$$a(j,j-1) = 0.5\pi Rtube^2(r_{j-1}^2 - r_{j-2}^2)Sp/Vp \qquad (22)$$

At first glance this may seem inconsistent within the AFM context--that the bed can be represented by solid and void spaces whose outlines determine the flow pattern. But although the solids are considered to have definite boundaries they are porous media so that the available surface area is actually greater than the overall shape would imply. This is similar to utilization of BET surface area for porous catalysts.

Note that the effect of pellet shape on these area parameters is implied by the term Sp/Vp. For spheres, Sp/Vp=6dp and for cylinders Sp/Vp=4dp.

Main Solid Plug

The solid element shown in Figure 22-b receives heat from the fluid above, conducts heat radially inward and then loses heat to the fluid below. This model assumes that axial temperature gradients within the solid are negligible in comparison to radial gradients. Thus, at any given z the steady-state heat balance becomes

$$t_{out} - t_{in} = R_{tube}\, r_{j-1} q \ln\left[\frac{r_j}{\lambda_s r_{j-1}}\right] \tag{23}$$

where q is the amount of heat transferred through the solid, and λ_s is the solid thermal conductivity. Note that q, Rtube, and λ, must be in a consistent set of units (e.g., CGS, MKS, etc.). But in the steady-state, heat in equals heat out, or

$$\begin{aligned} q &= h_p a(j,j+1)\,[T_{j+1} - t_{out}] \\ &= h_p a(j,j-1)\,[t_{in} - T_{j-1}] \end{aligned} \tag{24}$$

Combining these two equations leads to

$$t_{in} = \frac{T_j + (A^*+B)T_{j-1}}{1+A^*+B} \tag{25}$$

$$t_{out} = \frac{A^*T_{j-1} + (1+B)T_{j+1}}{1+A^*+B} \tag{26}$$

where

$$A^* = a(j,j-1)/a(j,j+1) \tag{27}$$

$$B = Rtube\; r_{j-1} hp\; a(j,j-1) \ln\left[\frac{r_j}{\lambda, r_{j-1}}\right] \tag{28}$$

Because the total heat transferred is small, B<<1 (see note, below) so that the solid has a flat radial profile at any given z, i.e. $t_{out} = t_{in} = t_j$. And, since half of the solid area faces up and half

down (equation (22)) A*=1 and t_j is the average of the two surrounding fluid temperatures:

$$t_j = \frac{1}{2}(T_{j+1} + T_{j-1}) \tag{29}$$

(Note: B<<1 can be justified by substituting typical values into equation (28). Suppose r_j=0.6, r_{j-1}=0.5, r_{j-2}=0.4 Rtube=3.6cm, hp=.001cal/s-cm^2-K, and the spherical pellets, dp=.26cm, are glass so that λ = .0029cal/s-cm-K.) This yields a(j,j-1)=1.83cm and B=.02.

Center Solid Plug

The arguments here follow those for the main solid plug. But, since the solid is completely surrounded by a single fluid plug (Figure 22-c)

$$t_1 = T_2 \tag{30}$$

Note that this is analogous to the Fickian boundary condition of zero temperature gradient at the tube centerline.

Center Fluid Plug

In this case, the fluid element (Figure 22-d) gains heat from the surrounding solid and from bulk inflow and loses heat to bulk flow only (no inner solid), so that

$$\rho C_p Q_1 \frac{dT_1}{dz} = hp\ a(1,2)[t_2 - T_1] \tag{31}$$

Wall Fluid Plug

Here, the fluid element (Figure 22-e) gains heat from the wall and from inflow and loses heat to outflow, so that

$$\rho C_p Q_N \frac{dT_N}{dz} = 2\pi Rtube\ hw[Twall-T_N]$$

$$-hp\ a(N,N-1)\,[T_N - t_{N-1}] \qquad (32)$$

where Twall is the wall temperature (constant).

Wall Solid Plug

A solid plug in contact with the wall as shown in Figure 22-f gains heat from the wall across a stagnant film, transfers radially inward via conduction and then loses heat across a pellet film resistance to the fluid at T_{N-1}. Within the solid itself, equation (23) for the main solid plugs holds but equation (24) must be replaced by

$$q = h^*a(s,w)\,[Twall - tout]$$

$$= hp\ a(N,N-1)\,[t_{in} - T_{N-1}] \qquad (33)$$

where h* is the stagnant wall film coefficient and a(s,w) is the area available for heat transfer across the stagnant film per unit length. Combining (23) and (33) yields

$$t_{in} = \frac{Twall + (A^{**}+B)\ T_{N-1}}{1+A^{**}B} \qquad (34)$$

where

$$B = Rtube\ r_{N-1} hp\ a(N,N-1) \ln\left(\frac{1}{r_{N-1}}\right)^{\lambda_s} \qquad (35)$$

Again, because the total amount of heat transfer is small (hp very low) B-->0 so that

$$t_{in} = \frac{Twall + A^{**}\ T_{N-1}}{1+A^{**}} \tag{36}$$

implying that the solid temperature is some weighted average of the wall and fluid temperatures. For the cases considered in the "Comparison with Experiment" section, it was assumed that

$$t_N = 0.1\ Twall + 0.9T_{N-1} \tag{37}$$

where the 0.1 and 0.9 weighting factors were found empirically to best fit the base case data. In retrospect, these weights can be justified somewhat by physical reasoning.

The moving stream below the solid plug should induce better heat transfer than the stagnant between the solid plug and the tube wall, so that hp>h*. And, the stagnant film heat transfer area a(s,w) (not well-defined from system geometry) may range from a(N,N-1) down to some fraction of πDt, so that a(s,w)<a(N,N-1) and hence A**>1. Note that if a(s,w)~a(N,N-1) and h*=(.1)hp then equation (36) yields weighting factors of 0.09 and 0.91 (as opposed to the 0.1 and 0.9 of equation (37)). Thus, although h* and a(s,w) cannot be ascertained from system geometry, the empirically derived weighting given by equation (37) seems reasonable.

Condensation of Equations and Solution Techniques

Description of the complete radial profile at any given z within an A-half-cell requires equations (30), (29) with j=3,5,...,N-1, (20) with j=2,4,...,N-2 and (32). (In this section N=Nrad, or the total number of plugs in any half-cell.) Equations (29) with j=2,4,...,N-2, (37), and (20) with j=3,5,...,N-1 and (32) are required for a B-half-cell. Since the temperatures vary with z, these equation sets must be integrated from plug inlet to outlet before mixing calculations can be made. After the cells and plugs are sized according to Dt/dp and ϵ_{bed} and the flows subdivided and mixing matrices determined as outlined in the mass dispersion chapter, the temperature profile at any given axial position can be obtained in the following manner:

1. set all inlet temperatures (solid and fluid) to Tin.
2. within the A-half-cell, integrate equations (32) and (20) for j=2,4,...,N-2 from z=0 to z=0.816dp (the length of one half-cell). Note that this must be done numerically as the interdependence of the equations precludes analytical results. At each integration step, obtain new solid temperatures via equations (30) and (29) for j=3,5,..., The outlet fluid temperatures (T_2, T_4,...,T_N) becomes the elements of the (N/2)-long vector TA(out,n), where n is the current cell number.
3. calculate the next B-half-cell inlet temperatures via the previously-defined mixing matrix, R used in the mass dispersion calculations:

$$\underline{TB}(in,n) = \underline{\underline{R}}\ \underline{TA}(out,n) \qquad (38)$$

where

$$\underline{TB}(in,n)^T = [T_1 T_3 \ \cdots\ T_{N-1}]$$

4. integrate equations (31) and (20) for j=3,5,...,N-1 from B-half-cell inlet to outlet, calculating new solid temperatures at each integration step (equations (37) and (29) for j=2,4,...,N-2). The outlet fluid temperatures ($T_1, T_3, \ldots T_{N-1}$) becomes the elements of the (N/2)-long vector $\underline{TB}(out,n)$.

5. calculate next A-half-cell inlet temperatures via the previously defined mixing matrix, $\underline{\underline{S}}$ used in the mass dispersion calculations:

$$\underline{TA}(in,n+1) = \underline{\underline{S}}\ \underline{TB}(out,n) \qquad (39)$$

6. repeat steps 2-5 until the desired number of axial cells has been traversed.

Model Parameters

Of the parameters necessary for heat but not mass dispersion, a(j,j+1) is defined by the AFM in terms of packing geometry (equation (22)) and a(s,w) and h* (equation (36)) are incorporated into the weighted average of equation (37). The nature of the coefficients hp and hw, on the other hand, prevents them from being determined solely by geometry. In fact, previous studies of flow around submerged objects (e.g. Bird et al., 1960) and in empty tubes (e.g., McCabe and Smith, 1976) show that film coefficients must

be correlated to system variables such as pellet or tube size, total flow rate, friction factor, and fluid properties (e.g., thermal conductivity and specific heat). The AFM thus draws on this experience to obtain general correlation forms for hp and hw. Experimental data are needed to determine some of the coefficients.

Pellet Film Coefficient (hp)

Forced-convection heat transfer from a single sphere in an infinite fluid moving at velocity v* has been related by Ranz and Marshall (1952)(Bird et al., 1960, p. 409) to system parameters via

$$\frac{hp\ dp}{\lambda_{fluid}} = 2.0 + \left(\frac{Cp\ \mu}{\lambda_{fluid}}\right)^{1/3} \left(\frac{dp\ G}{\mu}\right)^{0.5} \tag{40}$$

where λ_{fluid} = fluid thermal conductivity, $G=\rho v^*$, ρ = fluid density, C_p = fluid specific heat and μ = fluid viscosity. At high flow rate, the second term on the RHS of equation (40) will dominate, yielding, for a fluid with constant physical properties,

$$hp = K'\left(\frac{G}{dp}\right)^{0.5} \tag{41}$$

where K' is a constant.

For long cylinders of diameter dp with v* perpendicular to the axis, Bird et al. (1960, p. 408) also give a graphical correlation from Sherwood and Pigford (1952) of hp which can be represented by

$$\frac{hp}{G\ cp}\left(\frac{cp\ \mu}{\lambda_{fluid}}\right)^{2/3} = 0.42\left(\frac{G\ dp}{\mu}\right)^{-0.46}$$

which yields, for a fluid with constant physical properties

$$hp = K''\frac{G^{0.54}}{dp^{0.46}} \simeq K''\left(\frac{G}{dp}\right)^{0.5}$$

where K" is a constant, not necessarily equal to K'. Note that the interstitial value of G should be used for packed beds to account for the effect of overall bed voidage on velocity.

According to these relationships, then, hp should vary as $(G/dp)^{0.5}$ whether the pellets are spherical or cylindrical. Schlunder (1978) also notes that the single-pellet dependence of Nu ($Nu=hpdp/\lambda_{fluid}$) on the square root of Re_p should hold for packed beds if it is enhanced to account for the extra turbulence. The use of a single hp correlation form simplifies use of the AFM. However, pellet shape will influence the relative magnitude K'/K" as follows. Consider the random packing of cylinders versus spheres into a tube. Because spheres have no "corners" the fluid moves around hydraulically smooth surfaces. But, depending on their orientation, cylinders may offer surfaces of smoothness similar to spheres (v* perpendicular to pellet axis) or surfaces inducing maximum turbulence (v* parallel to pellet axis). And, at any angle in between the fluid must pass over some sort of corner. Thus, one can reason

that the increased turbulence through cylindrical (versus spherical) packing would lead to higher hp for the same G and dp.

Wall Coefficient (hw)

Forced-convection heat transfer in empty tubes has been related in many forms to system parameters (e.g., Bennett and Myers, 1982; Greenkorn and Kessler, 1972; McCabe and Smith, 1976). McCabe and Smith (1976), for example, give the correlations for smooth and rough pipes shown in Table 6. Note the dependence of hw on tube length in the first four relationships; this is probably due to the entrance effect discussed earlier. Thus, the AFM uses the fifth equation of Table 6 as a guide for a general form of correlation between hw and other system parameters.

The relationship f versus Re and relative roughness, (δ/Dt) in pipes is well-established (e.g., Greenkorn and Kessler, 1972, p. 226). Each (δ/Dt) establishes a separate curve (with f decreasing as Re increases) which can be represented by several segments over which

$$f = K_f/Re^n \tag{43}$$

where K_f is a constant. For smooth pipes, n is essentially constant, whereas for rough pipes n is maximum at low Re and equal to zero at "complete turbulence." The Re above which n=0 decreases as (δ/Dt) increases. The value of n also decreases as (δ/Dt) increases. Since trends in hw are desired, equation (43) can be combined with the fifth relationship of Table 6 to give (for ϕ(f)=1)

Table 6

Correlations for Forced Convection in Empty Tubes

1. Laminar Slow (GDt/μ= Re < 2100)

$$\frac{hwDt}{\lambda} = K_{\ell}\left(\frac{G\ Cp}{Dt^2 \lambda L}\right)^{1/3}$$

where K_{ℓ} is a constant and L is tube length

2. Transition flow (2100 < Re < 10000)

$$\frac{hw}{Cp\ G} = K_{tr}\left(\frac{Dt}{L}\right)^{1/3}\left(\frac{Dt\ G}{\mu}\right)^{-2/3}\left(\frac{Cp\ \mu}{\lambda}\right)^{-2/3}$$

where K_{tr} is a constant, L is tube length

3. Turbulent flow (Re > 10000)

$$\frac{hw}{Cp\ G} = \frac{K_{tu}\left(\frac{Cp\ \mu}{\lambda}\right)^{-2/3}\left(1 + \frac{Dt}{L}\right)^{0.7}}{\left(\frac{Dt\ G}{\mu}\right)^{0.2}}$$

where K_{tu} is a constant and L is tube length

4. Smooth Pipes (Re > 50000)

$$\frac{hw}{Cp\ G} = K_s\left(\frac{Cp\ \mu}{\lambda}\right)^{-2/3} f$$

5. Any Re

$$\frac{hw}{Cp\ G} = \frac{f}{\phi(f)}$$

where f is the friction factor and $\phi(f)$ is some function of f.

Compiled from McCabe and Smith (1976)

$$hw = K_f c_p G Re^{-n} \tag{44}$$

Hence, for a fluid with constant physical properties

$$hw = \frac{Kw\ G^{1-n}}{Dt^n} = \frac{Kw\ G^m}{Dt^n} \tag{45}$$

Note that interstitial values of G should be used here to account for the effect of overall bed voidage on velocity. The following trends should be expected in fitting hw to data via equation (45):

1. constant m for smooth pipes over a wide range of flow rates--m should be higher for rough tubes than for smooth ones, all else being equal;
2. increasing m as G increases--if the range of flow rates is large enough, several different m-values may be needed;
3. increasing m as Dt decreases--that n decreases as (δ/Dt) increases implies n is directly proportional to Dt for a given material with constant δ; hence, m=1-n is inversely proportional to Dt.

Other Parameters Influenced by Pellet Shape

To solve the AFM equations, the cells and plugs must be sized according to Dt, dp and ε_{bed} so that the flow rates and mixing matrices can be determined. The mass dispersion cases established these parameters for spherical packing, where radial and axial porosity profiles showed oscillations about ε_{bed} with cycle widths of 0.816 dp. But, one may question whether similar patterns would occur with cylindrical pellets.

The bed porosity, ε_{bed}, for cylindrical packing is lower than that for spherical packing of the same Dt/dp, if dp for each pellet is taken to be that of a sphere which would occupy the same volume (Leva and Grummer, 1947b; Roblee et al., 1958; Schwartz and Smith, 1953). This implies that because of their irregular shape, more cylinders can pack within a given boundary. And, cylinders are asymmetric, so they can assume any number of orientations upon being poured into a tube. Roblee et al. (1958) report radial porosity profiles for beds packed with cylinders. The profiles indeed show oscillation about the lower ε_{bed}. However, no definite conclusions regarding the actual cycle width can be drawn from their work since they present profiles for only one Dt/dp. The reported data represent segments, or disks, one pellet diameter long. Because of the expected axial oscillations in porosity, one pellet diameter is too short to represent average bed values and too long to yield axial cycle widths. Indeed, the data show two distinct profiles, each with a different period of oscillation.

Schwartz and Smith (1953) also give radial porosity profiles, but the radial increments over which measurements were taken are too wide to reveal oscillatory behavior. These authors also present radial velocity profiles for cylindrical packing which should at least hint at the radial oscillations in porosity. However, as discussed earlier, the measurements were made at only five radial positions in the empty tube some distance beyond the packed section and may not be truly representative of the packed bed itself. And,

Lerou and Froment (1977) showed that velocity measurements could be distorted simply by rearranging the last layer of pellets.

Consider again the orientation of cylindrical pellets into a tube. If it is assumed that the perpendicular (pellet axis at right angle to flow direction) and parallel (pellet axis parallel to flow direction) orientations are equally probable, then the fluid can encounter a barrier of width d or l with equal probability. Thus, the AFM uses the geometric mean

$$dp = \left(\frac{d^2 + l^2}{2}\right)^{0.5} \tag{46}$$

as the effective pellet diameter. Calculating dp in this way assures that if d=l, dp=d whereas the equivalent volume argument leads to

$$dp = (1.5)^{0.33}d$$

regardless of the aspect ratio d/l. The relationships presented for spherical pellets then use of the dp of equation (46) (and the corresponding Dt/dp) together with the lower ε_{bed} to determine axial cell length and radial plug width as presented for the mass dispersion cases. The individual flows and weighting matrices follow accordingly. (Note that if ε_{bed} is not measured but instead determined from the data of Leva and Grummer 1947b dp=d/4 should be used to calculate Dt/dp in using their graphs--but not in AFM equations--since that is the manner in which their data are presented.)

Determination of Film Coefficients

The previous section established that hp should be proportional to the square root of (G/dp) (equation (41)) with hp for cylindrical pellets excess hp for spherical pellets under equal conditions. This in turn implies that if hp is known at one G/dp or "base case" for a given packing (e.g., smooth spheres, rough spheres, smooth cylinders, etc.) the hp at any other G/dp combination can be determined from

$$hp = hp_{base}\left[\frac{Gint}{Gint,\ base}\ \frac{dp,\ base}{dp}\right]^{0.5} \qquad (48)$$

where $$Gint = \frac{\rho Q}{\varepsilon_{bed} Atube}$$

It was also established that hw should vary as G^m where m depends on system variables such as tube diameter, pipe material and degree of turbulence (i.e., range of G). Since turbulence in packed beds cannot be readily defined (refer to earlier discussions of particle- and hydraulic-Re in the mass dispersion chapter), the value of m cannot be specified a priori but must be fit to data for a given set of system variables (Dt, pipe material) over the desired range of flow rates. While this may at first seem dissatisfying, note that since hp is predetermined according to a base case, hw remains the sole parameter to be correlated. The power-law expression for hw (equation 45))

is simple to work with. Also recall that no single correlation for hw exists even for forced-convection in empty tubes due to the complex nature of turbulence. (This may also be the reason that so many correlations exist for the hw used in conjunction with the Fickian analogy.)

To adequately fit these parameters several types of data are desired:

1. bulk-average outlet fluid temperature, Tb, out--to indicate the total amount of heat transferred,
2. radial temperature profiles--to indicate radial dispersion of heat; temperature at one ratial position other than wall (e.g., tube centerline) should suffice if used in conjunction with Tb, out,
3. axial temperature profiles--to support the argument that hw should be constant for packed beds since the turbulence never dies out.

These data types are listed in order of preference. That is, Tb, out is the most preferred because its measurement is accurate and straightforward. And, since the AFM will most likely be unable to attain a "perfect fit," radial temperature profiles cannot be used without knowledge of the flow distribution at the measurement point to determine Tb, out. Most of the flow within a packed bed channels towards the tube wall so that fluid temperatures closest to the wall should be weighted most heavily. But if the temperature profiles are measured in the empty tube some distance beyond the packed section judgment must be used in weighting the individual radial temperatures to determine

Tb, out. (Recall from earlier discussion that the radial distribution of flow rate changes as the fluid exits the packing.) And, axial temperature gradients at a single radial position alone provide too little information to correlate hw.

To correlate hp and hw for the AFM a base case must first be chosen. The system should contain the fewest possible unknowns. It should have spherical packing to eliminate uncertainties regarding flow and porosity profiles and pellet shape. The pellets should be smooth to eliminate uncertainties regarding surface roughness. The tube should be made of a smooth material so that the exponent m (equation 45)) will be constant over a large range of flow rates. Within this system, a single experiment is designated as base case for which hp and hw are determined by trial and error to give the best Tb, out and radial and axial temperature profiles. This value of hp is used as hp, base in equation (48) and the corresponding flow rate, bed porosity and pellet size yield Gint, base and dp, base.

After the base case has been established, the functional forms of equations (48) and (45) can be verified by changing dp and G. Note that changes in Dt/dp may effect ϵ_{bed} which must then be incorporated in the value of Gint. The coefficient hp is predetermined by equation (48) but hw must be best-fit to each new experiment.

If the tube is hydraulically smooth (e.g., glass or brass, Bennett and Myers, 1982) one can verify the heat transfer/friction factor analogy implied in equation (45) by comparing the value of m predicted for empty tubes to that needed by the AFM in equation (45). For smooth

empty tubes, m should be constant over a wide range of Re (flow rates) (see, for example, Greenkorn and Kessler, 1972, pg. 226). Curve-fitting the empty tube value of f at Re=60,000 and 250,000 leads to

$$4f = 0.184\ Re^{-.202}$$

(These values of Re have no significance other than convenience in reading the f-Re graph.) Thus, n=0.2 and m=0.8 (equation (45)) so that

$$hw = hw,base \left(\frac{Gint}{Gint,\ base} \right)^{0.8} \tag{49}$$

should hold for smooth tubes. Stretching the analogy further would imply that experiments carried out in rough tubes should lead to m>0.8.

The hypothesis that pellet shape would effect the magnitude, but not functional form of hp can be tested by letting

$$\begin{aligned} hp &= \gamma\ hp,\ sphere \\ &= \gamma\ hp,\ base \left(\frac{Gint}{Gint,base} \frac{dp,base}{dp} \right)^{0.5} \end{aligned} \tag{50}$$

where γ is a constant that accounts for enhanced heat transfer due to increased turbulence from non-smooth or asymmetric pellets. For cylindircal pellets, then, a new base case must be selected and the coefficients hp and hw again fit by trial and error. The constant γ can then be back-calculated from equation (50). For the hypothesis

to be valid, γ should exceed one but should remain constant for all systems employing cylindrical pellets.

Comparison with Experimental Data

This section presents AFM heat dispersion results for beds packed with uniformly sized spherical or cylindrical pellets. Model parameters are related to the framework within which they were developed--submerged object form for hp (equations (48) and (50)) and friction factor analogy for hw (equation (45)). In general, AFM resulta are not compared to the Fickian analogy because the large number of correlations available for pertinent parameters (as discussed at the beginning of this chapter) would yield a wide range of solutions to equation (19). However, where appropriate, comparisons with back-fit Fickian model may be made.

It should be noted in reading this section that the AFM uses interstitial mass fluxes, Gint, to account for the effect of overall bed voidage on velocity. Any G's attributed to other researchers represent superficial values.

Yagi and Wakao (1959) give both centerline and bulk-average outlet temperatures for their experiments in a (smooth) brass tube packed with smooth, uniformly sized glass pellets. They used one tube size with two different pellet sizes over a range of particle-Reynolds numbers $100<Re_p<700$. For their "F-1" run (G=2740 kg/hr-m^2, Dt=3.6cm, dp=.6 cm) they also give the axial variation in centerline temperature. This was therefore selected as the base system with run F-1 as the base case.

Figure 23 compares AFM results (hp,base=.002 cal/s-cm^2-K hw,base=.002 cal/s-cm^2-K) and best-fit Fickian profile and Tb, out to data for the base case. Table 7 compares AFM and best-fit Fickian results to outlet centerline and bulk-average temperature data for all other "E" (dp=0.26cm) and "F" (dp=0.6) runs with hp determined from equation (48) and hw from equation (49), i.e. equation (45) with m=0.8. In predicting bulk outlet values, the AFM surpasses the Fickian analogy in all but three of the cases (in two of these, it differs from the Fickian back-fit by only 0.2^{o}C). In predicting outlet centerline temperatures, the AFM again surpasses the Fickian back-fit in all but three cases (in two of these, the AFM prediction of the corresponding Tb, out is within 0.2^{o}C of the Fickian back-fit). The worst AFM fit is for the centerline temperature of the Rep=106 case. But, recall from earlier discussion that the relationship given by equation (48) is a simplified version of equation (40); it presumes that flow rate is high enough to dominate the RHS of equation (40). If the flow rate, or Re_p, is low, the constant term may begin to assert itself, i.e., the hp based on the complete version (equation (40)) would be larger than hp determined from the simpler version (equation (48)) (For example, the AFM can better fit the data with the same hw and higher hp--at 1.2 times the value used in Table 7 -- to give: (1) centerline temperature of 63.4^{o}C (AFM) versus 65.3^{o}C (data); and (2) Tb, out of 78.8^{o}C (AFM) versus 77.3^{o}C (data).) Further, Table 7 notes that the AFM must distribute the flow according to the laminar/transition, rather than turbulent, hydraulic resistances. The mass dis-

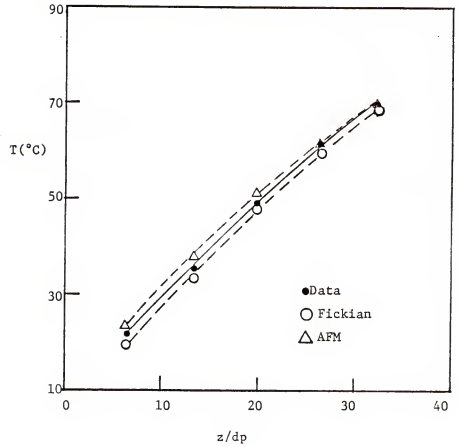


Figure 23: Axial Temperature Profiles for Re_p=234, Dt/dp=6.0, Data of Yagi and Wakao[P] (1959)

Table 7

AFM for Heat Dispersion in Smooth Brass Tube Packed With Glass Spheres

d_p (cm)	Re_p	Item (at exit)	Data	AFM[a]	Fickian[b]
0.6	234	t_c	69.8	69.9	68.5
		T_b	78.8	78.1	77.9
0.6	382	t_c	63.6	62.3	62.1
		T_b	74.8	71.7	73.8
0.6	691	t_c	56.1	57.8	54.1
		T_b	69.2	67.9	67.7
0.26	106[c]	t_c	65.3	60.2	64.0
		T_b	77.3	77.8	76.4
0.26	183	t_c	51.3	49.4	50.1
		T_b	69.7	70.4	69.0
0.26	238	t_c	52.1	48.8	49.7
		T_b	68.1	69.9	66.5
0.26	323	t_c	50.1	48.2	47.9
		T_b	67.1	69.3	65.5

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a. AFM predictive; used ε_{bed}~0.40 in all calculations
b. Fickian back-fit; parameters specified in Table 8
c. AFM used laminar/transition hydraulic resistances to radially distribute flows.

All data from Yagi and Wakao (1959); air at inlet near T_{in}=20°C; Twall=100°C, Dt=3.6cm in all cases.

Table 8

Fickian Parameters for Table 7 Experiments of Yagi and Wakao (1959)

		(1000hw)(cal/s-cm^2-K)		(1000λe,r)/(cal/s-cm-K)	
(cm)	Re_p	back-fit[a]	correlated[b]	back-fit	correlated[b]
0.6	234	1.81	1.65	1.52	1.53
0.6	382	2.52	2.44	2.00	2.22
0.6	691	3.61	3.92	3.04	3.68
0.26	106	2.02	2.02	1.25	1.03
0.26	183	2.85	3.13	1.41	1.48
0.26	238	2.88	3.86	1.93	1.79
0.26	323	3.66	4.93	2.35	2.29

a. Back-fit by Yagi and Wakao (1959); assume $K_{air} \sim 70 \times 10^{-6} \frac{cal}{s\text{-}cm\text{-}K}$

b. From correlation given by Yagi and Wakao (1959); $Pr_{air}=0.75$
The correlation for λe,r (Their equations 4 and 5) suggests $(\alpha\beta)_H=0.09$ for Cp=0.6 and 0.11 for dp=0.26

persion chapter states that this is necessary at Re_p<150, implying that Re_p --while not the sole parameter dictating packed bed turbulence--must give some indication as to flow regime. It is therefore possible that at this low Re_p=106 the hw exponent m (equation 45)) may not be 0.8. Even for smooth pipes, the f-Re curve has distinct regions for laminar and turbulent flow. For this reason and because only one heat dispersion data set was available at Re_p<150, the hp values were not fit to the complete form (equation (40)).

According to these arguments, then, the use of equation (48) to determine hp is justified. And the fact that m=0.8 for hw correlates the data so well justifies not only the form of hw given by equation (45) but also the friction factor ananlogy. Recall from the previous section that m=0.8 was predicted solely from arguments relating heat to friction factors in empty tubes (equation (49)). It should be noted that Yagi and Wakao also found hw to vary as $G^{0.8}$ in correlating the Fickian analogy to their experiments.)

Other systems for which the literature provides the actual temperature data needed to correlate AFM parameters are summarized in Table 9. This table excludes any systems containing pellets of high thermal conductivity (e.g., Baumeister and Bennett, 1958; Colburn, 1931; Kwong and Smith, 1957) since the AFM presumes no conduction between pellets, and it excludes any systems of highly irregular geometry, i.e., annular or other non-circular tubes (e.g., Wakao and Kato, 1969; Yagi and Kunii, 1960) or packing made up of anything but uniformly

Table 9 Available Temperature Data

Source	Pellet shape[a]	Pellet d_p[b]	Pellet material	Tube Dt	Tube material	Re_p range
Yagi and Wakao (1959)[c,d]	s	0.26cm -0.6cm	glass	3.6cm	brass	100 -1.700
Leva (1947)[c,d]	s	0.172cm - .388cm	glass	2cm and ½ cm	standard	2 -850
Leva and Grummer (1948)[d,e]	s,c	varied	glass and rough	2cm and 3/4cm	standard	n.a.[j]
Plautz and Johnstone (1955)[f]	s	1.82cm	glass	20.6cm	?	n.a.[j]
Bunnell et al. (1949)[f,g]	c	1/8cm	alumina	2cm	?	n.a.[j]
Hall and Smith (1949)[f,g]	c	1/8cm	alumina	2cm	?	n.a.[j]
Calderbank and Pogorski (1957)[h]	c,s	1/8cm -1/2cm	various	4cm	?	n.a.[j]

Table 9-continued

Source	Pellet shape[a]	Pellet dp[b]	Pellet material	Tube Dt	Tube material	Re_p range
Lerou and Froment (1977)[d,i]	c	0.95cm	V_2O_5 catalyst	9.9cm	?	120-500
deWash and Froment (1972)[i]	c	0.57cm	"	15.75cm	?	n.a.[j]
Schortz and Bischoff (1969)[h,i]	s	0.3cm	stoneware	4cm	?	n.a.[j]
Coberly and Marshall (1951)[d]	c	3/8cm x 1/2cm	celite	5cm	?	360-1300

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a. s→spherical; c→cylindrical

b. If cylindrical, see individual reference for definition of dp

c. other shapes and materials; centerline profile for one run; centerline and T_b at outlet for all other runs.

d. authors also studied other Re_p and/or pellets of other shapes, sizes, or materials but these additional data not used, for comparison here.

e. beds packed with mixtures of pellet sizes; thus, data not compared herein because of uncertainty in bed porosity characteristics.

Table 9-continued

f. non-uniform inlet temperature profile (radial) which was not clearly specified; not enough data to back-out full $T_{in}(r)$ description;

g. screens located at several axial positions to guide thermowells; thermowells inserted through entire bed length at several radial positions; natural packing pattern disturbed and porosity profiles $\varepsilon(r,z)$ unknown;

h. unclear which systems correspond to data presented;

i. tempeatures measured more than ldp beyond packed section

j. not applicable; data not used for comparison.

sized spheres or cylinders (e.g., Leva and Grummer, 1948). Some systems of the desired geometry were also rejected for purposes of AFM correlation for other experiment-related reasons as noted in Table 8.

Whereas Yagi and Wakao (1959) used smooth brass tubing, the other researchers listed in Table 8 used "standard" pipe, which is probably rougher than brass (e.g., Bennett and Myers, 1982). Thus, these systems should yield higher m values in the hw correlation and may exhibit several flow rate regimes over which m can be considered constant. Only Tb, out data are available for the spherical systems (other than Yagi and Wakao, 1959), as noted in Table 8. While Tb, out provides sufficient information with which to correlate hw (recall discussion in previous section) the absence of radial or axial temperature profiles prevents double-checking the goodness of fit. But, the form of equation (45) implies that a log-log plot of hw versus G should provide a straight line of slope m. The degree of scattering over small segments of G should indicate the adequacy of the correlation. A distinct change in slope at high or low G would indicate that the system has moved from one f-versus-Re regime to another.

Such log-log plots of AFM hw versus flow rate for smooth glass spherical packing in standard pipe (Leva 1947a) are shown in Figure 24 for the smaller tube (Dt=1.58cm, Dt/dp=4.95, runs 100a-e) and in Figure 25 for the larger tube (Dt=5.26cm, Dt/dp=5.33, runs 9a-h). Each plot shows a definite straight line segment with the expected change in slope (m not constant for all G in rough tubes) and with essentially no scatter in the constant slope segment. The values of m=1.0 for the

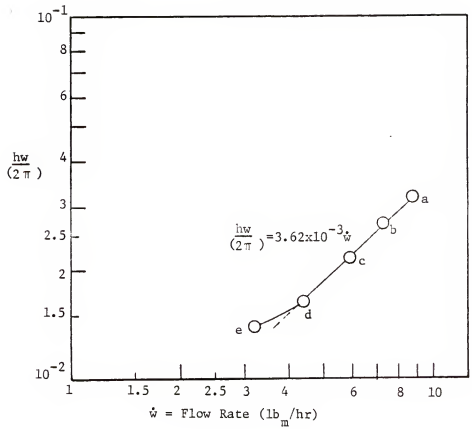


Figure 24: AFM Wall Film Coefficients for Data of Leva (1947b), Runs 100a-e, Dt/dp=4.95, Dt=1.6cm

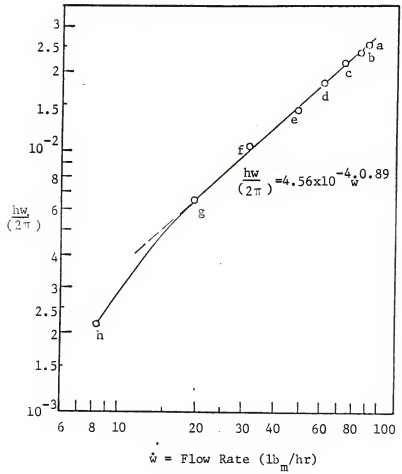


Figure 25: AFM Wall Film Coefficients for Data of Leva (1947b), Runs 9a-h, Dt/dp=5.33, Dt=5.3cm

tube and m=0.89 for the larger tube are consistent with the friction factor analogy discussed earlier: for tubes of the same material, m should be inversely proportional to Dt.

The available literature data for cylindrical pellets provide only radial temperature profiles (albeit at several bed depths for Coberly and Marshall, 1951) without corresponding Tb, out values. Fitting hw to data of this type presents some difficulty as the distance between temperature measurement point and bed exit increases. Unless the temperatures are actually measured inside the packed section, the difficulty in fitting hw would also increase as the bed length increases. Consider the following arguments.

As the fluid exits the packed section it mixes radially as it expands from the packing interstices into the empty tube. As the fluid moves further into the empty section, its flow tends to redistribute from the maximum-near-wall profile characteristic of packed beds to the maximum-near-wall profile characteristic of empty tubes. Thus, at the bed exit, mixing occurs because of bulk fluid motion in the radial direction. This bulk mixing should in turn effect the temperature profile as the hotter fluid near the wall mixes with the cooler fluid near the centerline. This effect would be most dramatic when temperature profiles just inside the bed exit are the sharpest, i.e. for short beds. This exit effect may also cause difficulty in determining hp since it is the AFM's instigator of radial temperature gradients.

Furthermore, Lerou and Froment (1977) and deWasch and Froment (1972) observed "humps" in their measured radial temperature profiles. These humps were most pronounced for short beds and tended to disappear as bed length was increased. That these humps may be results of the measurement exit effect is further supported by the ability of deWasch and Froment to find a point for temperature measurement beyond the packed section after which the humps disappeared.

Coberly and Marshall (1951) ran their experiments with the thermowells "...nearly touching the packing." They also measured radial profiles at several bed depths, keeping all other system variables constant. Thus, if hw and hp are fit to their data at maximum bed depth, the corresponding AFM predicted axial-radial temperature profiles can be compared to data to provide added insight into the goodness of fit. These researchers studied several system geometries, but the system of 3/8" x 1/2" cylinders packed in a 5" tube was selected for AFM comparison since it provided the smallest Dt/dp. The geometric mean dp (equation (46)) for cylinders of this aspect ratio is 0.44" so that Dt/dp=11.3.

Figure 26 shows the log-log plot of AFM hw versus flow rate for this system and Figure 27 compares the corresponding AFM axial temperature profiles (at several radial positions) to experimental data. In Figure 26 note the constant slope segment breaking off at low flow rates, in accordance with the friction factor analogy. The high value of m=2 cannot, however, be explained within that framework. Note from

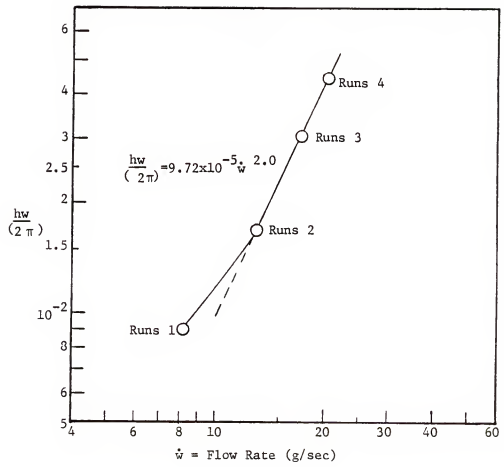


Figure 26: AFM Wall Film Coefficients for Data of Coberly and Marshall (1951), 3/8"x1/2" Cylindrical Pellets

Figure 27 how closely AFM results follow the axial temperature profiles. The largest deviations are at small r near z=0. But, as indicated on the Figure, the flow rates at these inner radii are small proportions of the total stream. Thus, those points with the largest absolute error in temperature will have the smallest relative contribution to the overall system. This factor becomes especially important in extending the AFM to include catalytic reactions.

In fitting hp and hw to temperature profiles for all four flow rates (at maximum bed depths, i.e., sequence number six in each run set) some judgment was needed in weighting the temperatures closest to the wall more heavily than others, as discussed in the previous section. Thus hw was fit for each case by trial and error BEFORE any plots were made to avoid bias towards the functional form of equation (45).

The constant, γ used to determine hp via equation (50) was determined from run 1-6 to be 1.33. This value of $\gamma>1$ is consistent with the idea that cylindrical pellets increase turbulence and enhance heat transfer over what would be expected for spherical pellets.

Figure 28 shows the log-log plot of AFM hw versus flow rate for the data of Lerou and Froment (1977) (Dt=9.9cm, cylindrical pellets with d=l=dp=0.95cm, bed length=48.8cm). This plot also shows consistency with the friction factor analogy as the constant slope of m=0.66 at low flow rate. The magnitude of $m<0.8$ cannot, however, be explained within the framework of the friction factor analogy. Since neither

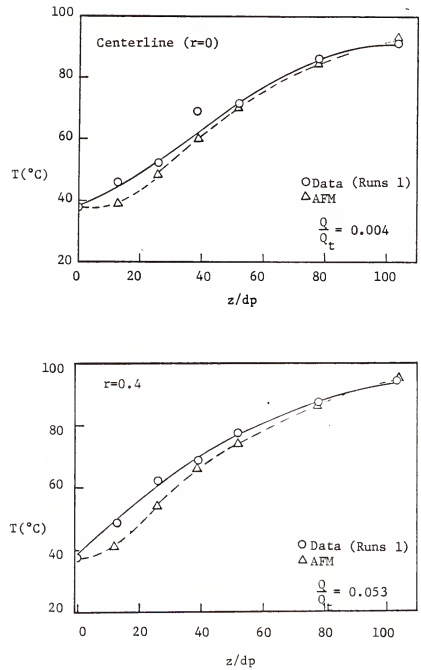


Figure 27: Axial Temperature Profiles for Data of Coberly and Marshall (1951), 3/8"x1/2" Cylindrical Pellets, at two Radial Positions

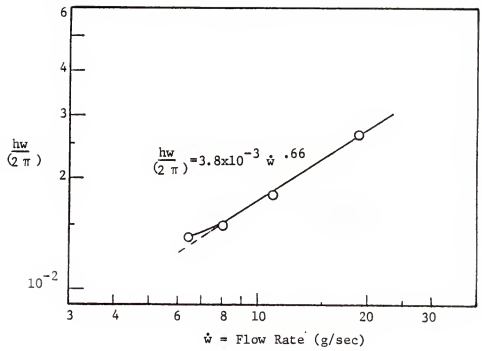


Figure 28: AFM Wall Film Coefficients for Data of Lerou and Froment

Tb, out values nor axial temperature profiles are available for these experiments, no further checking via data can be done. Here, as above, hp was calculated from equation (50) with γ=1.33 and hw was determined by more heavily weighting the outermost temperatures with the same precautions to avoid bias towards equation (45).

Note the slight scattering of points about the straight segment in Figure 28. The scattering may indicate deviation from the friction factor analogy or hw. Recall, however, the effect of thermowell placement on data accuracy when Tb, out is unavailable. Although Lerou and Froment give no specific axial location of thermowells, they state that their apparatus is similar to that used by deWasch and Froment (1972). In their experiments, deWasch and Froment located their thermocouples "...slightly above the packing, at a distance of one particle diameter. From this distance onwards, the radial temperature profile was completely smooth." In light of the earlier discussion regarding humps in the radial temperature profiles, this may imply that the flow redistribution causing the exit effect may already be complete by the time the measurement is taken. Thus, the AFM may have been fit to a temperature profile that is flatter than the one just before the end of the packed section. A flatter-than-actual profile would imply that the fluid had extra "time" to gain heat, i.e., that the effective flow rate was lower than actual. This may explain the low value of m=0.66 obtained for these experiments. For this reason, the AFM was not fit to the data of deWasch and Froment (1972).

Summary of AFM for Heat Dispersion

The Alternating Flow model presumes that heat disperses radially in packed beds through a film resistance at the tube wall and then through a series of pellet film resistances and that heat disperses axially as the fluid repeatedly splits and merges as it traverses many pellet layers. The AFM focuses on fundamental system parameters such as turbulence, pellet size and shape and tube characteristics. Of those AFM parameters needed for heat but not mass dispersion, only one, hw, must be back-fit for each new set of tube-related variables (e.g., tube material and diameter). This back-fitting is necessary because of the complex nature of forced-convection film heat transfer. The wall coefficient, hw, follows a friction factor analogy well, giving some insight as to how, in general, it will depend on other system variables. The friction factor/heat transfer analogy gained credibility as hw versus flow rate correlations took on the expected form. (Indeed, for the case of smooth tube material, the exponent m of equation (45) could be predicted solely from empty tube arguments.) The pellet heat transfer areas are determined from packing geometry (equation (22)). The pellet film coefficient, hp, correlated well to system variables via equation (48). This supports the presupposition that hp for pellets would correlate in the same general form as hp for a single pellet submerged in an infinite fluid.

In addition, the AFM gave good results for both cylindrical and spherical pellets. This justifies the correlation of hp by equation (50) (with γ=1 for spheres and 1.33 for cylinders). The good fit of

AFM to data for cylindrical pellets also justifies using a geometric mean pellet diameter (equation (46)) and the lower ε_{bed} expected for cylindrical packing in the porosity relationships for spherical packing. These relationships in turn determine flow distribution and mixing characteristics.

CHAPTER IV
REACTION

Previous chapters demonstrated the applicability of the Alternating Flow model to simple cases of heat and mass dispersion in packed beds. This chapter, therefore, extends the AFM to include catalytic reaction within the packing material. AFM equations for both adiabetic and wall-cooled reactors are developed and applied to example problems so that general AFM trends can be demonstrated. First-order intrinsic kinetics in the diffusion-limited regime are used. Unlike previous chapters, however, no comparison to actual data is made here. The intent of this chapter is to point out differences between the AFM and the Fickian analogy, thus laying the foundation for future work.

Model Development

The AFM views cases involving catalytic reaction as a combination of mass and heat dispersion steps. As the fluid moves through each radial plug, its reactant concentration decreases because of reaction to the surrounding solid plugs and its temperature increases due transfer of heat of reaction across a film from the solids. In general, the AFM obtains fluid concentrations and temperatures from the plug flow equation for each fluid plug and obtains solid temperatures from steady-state pellet heat balances. The AFM uses heat and mass

dispersion parameters developed in previous chapters and any required reaction-diffusion parameters (e.g., intrinsic kinetics and effective pellet diffusivity). In addition, the AFM also employs the assumptions customarily applied to reaction-diffusion problems (e.g., Lee, 1985; Carberry, 1976; Froment and Bischoff, 1979):

1. dominating external heat transfer resistance--isothermal pellet with all of the temperature drop across the external film,
2. negligible external mass transfer resistance--concentration at pellet surface equal to surrounding fluid concentration.

Any previously-stated AFM assumptions also carry over.

As in the heat dispersion chapter, each plug type must be treated separately:

1. main solid plug (e.g., plugs A3, A5, B2, and B4 of Figure 2)--each side subjected to a different concentration, thus a "two-sided" rate expression must be used; solid temperature obtained via steady-state film heat balance;
2. main fluid plug (e.g., plugs A2, A4, B3, and B5 of Figure 2)--surrounding solids at different temperatures, thus radial loss of reactants at two different rates; temperature rise due to heat transfer from both films;
3. center solid plug (e.g., plug A1 of Figure 2)--surrounded by single fluid annulus, so no need for "two-sided" rate expression; steady-state heat balance yields solid temperature;

4. center fluid plug (e.g., plug B1 of Figure 2)--surrounded by single solid annulus, thus only one rate needed; temperature rise due to heat transfer from film;
5. wall solid plug (e.g., plug B6 of Figure 2)--wall on one side and fluid on the other implies rate into fluid and no reaction at the wall; in wall-cooled reactor, heat transfer at wall requires inclusion of stagnant film wall coefficients h*, a(s,w) of Heat Dispersion chapter); adiabatic reactor implies symmetric boundary conditions and provides an expression similar to the one for the center solid plug;
6. wall fluid plug (e.g., plug A6 of Figure 2)--rate of reaction into solid below but not to wall above; heat transfers in across a pellet film resistance (hp) from below; and, for a wall-cooled reactor, out across a wall film resistance (hw) as described for the simple heat dispersion case; no wall heat transfer in the adiabatic reactor.

Throughout the following development, lower case t refers to solid temperature and upper case T to fluid temperature.

Main Solid Plug

Consider a solid plug with each face subjected to different conditions (Figure 29-a). For a catalyst with unsymmetrical concentration boundary conditions, the work of Tan and Smith (1980) for first order intrinsic kinetics

$$r_c = C\ k(t) = C\ k_o \exp(-g/t) \qquad (51)$$

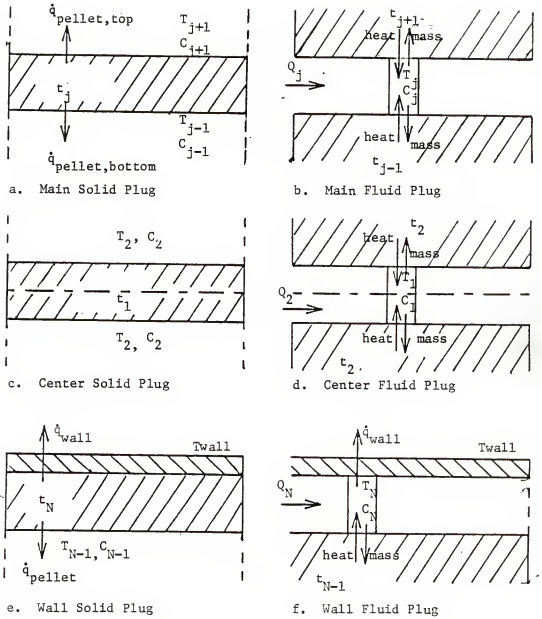


Figure 29: Plug Types for AFM Reaction Analysis

can be applied to give the molar flux, J_i, for diffusion-limited cases ($\phi>3$, $\phi=L(k/De)^{0.5}$):

$$J_i = C_i[\ De\ k(t)\ ]^{0.5} \tag{52}$$

where i = top or bottom, J_i is the molar flux (mol/cm^2) out the i-th face, C_i is the concentration of the key component (mol/cm^3) at the i-th face, De is the effective diffusivity of the key component in the catalyst and k is the rate constant evaluated at the pellet temperature. (Appendix H develops the rate expression for unsymmetric boundary conditions and more general intrinsic kinetics.) In the steady-state any heat generated by reaction is transferred across the pellet film resistance to give

$$\begin{aligned} &hp\ a(j,j-1)[t_j-T_{j-1}] + hp\ a(j,j+1)[t_j-T_{j+1}] \\ &= (-\Delta H)\ S'_p[C_{j-1}+C_{j+1}]\ [\ De\ k(t_i)\ ]^{0.5} \end{aligned} \tag{53}$$

where hp is the pellet film heat transfer coefficient (defined in the heat dispersion chapter), a(j,j+1) and a(j,j-1) are the corresponding heat transfer areas (also previously defined, equation (22)) and $(-\Delta H)$ is the heat of reaction. The heat dispersion chapter assumes that half of the pellet surface area faces up and half down (equation (22)) so that $a(j,j+1)=a(j,j-1)=S'_p$. Because the fluid temperatures are "known" at any position within the half-cell (e.g., at inlet from mixing calculations or elsewhere from integration of fluid

equations) equation (53) contains only one unknown: the pellet temperature. But, the exponential form of the rate constant prevents direct solution for t, so that "trial and error" must be used. If no solution is possible, i.e., the heating curve (RHS of equation (53)) does not intersect the cooling curve (LHS of equaiton (53)), the reaction is unstable.

For convenience, however, the rate constant can be linearized via a Taylor series (following Lee, 1981). Rearranging equation (53) gives

$$(t_j - T^*) = X' \, (k_o)^{0.5} \exp(-g/2t_j) \tag{54}$$

where

$$X' = (-\Delta H)[De]^{0.5} C^*/hp$$

$$T^* = (T_{j+1} + T_{j-1})/2$$

$$C^* = (C_{j+1} + C_{j-1})/2$$

since $a(j,j+1) = a(j,j-1) = Sp'$. Then, expanding the exponential in a Taylor series about T* and dropping quadratic and higher order terms gives

$$(t_j - T^*) = X \left[1 + (t_j - T^*)/2(T^*)^2 \right] \tag{55}$$

where

$$X = X' \, k(T^*)$$

or

$$t = T^* + \left[\frac{1}{\dfrac{hp}{(-\Delta H) C^* (De \, k(T^*))^{0.5}} - \dfrac{g}{2(T^*)^2}} \right] \tag{56}$$

Instability would be indicated by a negative RHS of equation (55).

Main Fluid Plug

A fluid element as shown in Figure 29-b can be described by

$$Q_j \frac{dC_j}{dz} = -[(Sp' J)_{j+1} + (Sp' J)_{j-1}] \tag{57}$$

and

$$\rho C_p Q_j \frac{dT_j}{dz} = hp\ a(j,j+1)[t_{j+1}-T_j] + hp\ a(j,j-1)[t_{j-1}-T_j] \tag{58}$$

where z is the distance into the half-cell, C_j is the key component concentration in the j-th radial plug, Q_j is the flow rate through the j-th radial plug, ρ is the fluid density, and C_p is the fluid heat capacity. The area parameters and pellet film coefficients were defined in the heat dispersion chapter. From equation (52)

$$\begin{aligned}(J\ Sp')_{j+1} &= Sp'_{j+1} C_j [De\ k(t_{j+1})]^{0.5} \\ (J\ Sp')_{j-1} &= Sp'_{j-1} C_j [De\ k(t_{j-1})]^{0.5}\end{aligned} \tag{59}$$

where Sp' is the catalyst surface area available for reaction at one face of a given solid plug. These areas were defined for heat transfer in Chapter III so that

$$\begin{aligned}Sp'_{j+1} &= a(j,j+1) \\ Sp'_{j-1} &= a(j,j-1)\end{aligned} \tag{60}$$

The solid temperatures are determined via equation (56). The complexity of equations (57) and (58) requires numerical integration from plug inlet to plug outlet.

Center Solid Plug

Figure 29-c shows that the center solid plug can be treated as

a single pellet surrounded by a fluid of concentration C_2. Thus, a symmetric effectiveness factor (e.g., Carberry, 1976) can be applied to give

$$J = C_2[\mathrm{De}\ k(t_1)]^{0.5} \tag{61}$$

A steady-state film balance leads to

$$hp(t_1-T_2) = (-\Delta H)\ C_2[\mathrm{De}\ k(t_1)]^{0.5} \tag{62}$$

if it is again assumed that $a(1,2) = Sp'_1$. Linearizing the exponential about T_2 yields

$$t_1-T_2 = \left[\frac{1}{\frac{hp}{(-\Delta H)C_2(\mathrm{De}\ k(T_2))^{0.5}} - \frac{g}{2T_2^2}}\right] \tag{63}$$

Again, instability would be indicated by a negative RHS of equation (63).

Center Fluid Plug

The description of the center fluid plug (Figure 29-d) contains only one reaction term:

$$Q_1 \frac{dC_1}{dz} = -Sp'_2\ C_1\ [\mathrm{De}\ k(t_2)]^{0.5} \tag{64}$$

and

$$\rho C_p Q_1 \frac{dT_1}{dz} = hp\ a(1,2)[t_2-T_1] \tag{65}$$

where, again it is assumed that $Sp'_2 = a(1,2)$. Both equations (64) and (65) must be integrated numerically with t_2 evaluated at each step via equation (56).

Wall Solid Plug

A solid plug adjacent to the tube wall (Figure 29-e) of an adiabatic reactor can be treated as half of a symmetric pellet (since there is no temperature gradient at the wall). In this case, the analysis follows that for the center solid plug to give

$$t_N - T_{N-1} = \frac{1}{\frac{hp}{(-\Delta H)C_{N-1}(De\ k(T_{N-1}))^{0.5}} - \frac{0.5\ g}{(T_{N-1})^2}} \qquad (66)$$

For a wall-cooled reactor, a stagnant film heat transfer resistance at the wall must be included:

$$(-\Delta H)Sp'_N C_{N-1}[De\ k(t_N)]^{0.5} = hp\ a(N,N-1)[t_N - T_{N-1}] + h^*\ a(s,w)[t_N - Twall] \qquad (67)$$

Dividing both sides by [hp a(N,N-1)] and using equation (60) gives

$$(-\Delta H)C_{N-1}[De\ k(t_N)]^{0.5} = [t_N - T_{N-1}] + \alpha[t_N - Twall] \qquad (68)$$

where

$$\alpha = h^*\ a(s,w)/hp\ a(N,N-1) \qquad (69)$$

The heat dispersion chapter showed that h* a(s,w)=0.1hp a(N,N-1) gave good results for the cases studied there. Thus, taking α=0.1 and linearizing the exponential of equation (68) about T_{N-1} gives

$$t_N = \frac{(X''Y-1)T_{N-1} - 0.1\ Twall - X''}{X''Y - 1.1} \qquad (70)$$

where

$$Y = g/[2\ T_{N-1}^2]$$

$$X'' = (-\Delta H)C_{N-1}[De\ k(T_{N-1})]^{0.5}/hp$$

Here, instability should be suspected if calculations lead to $t_N << T_{N-1}$ or to $t_N < Twall$. (If Twall is low enough, cooling may cause t_N to be lower than T_{N-1}.)

Wall Fluid Plug

A fluid plug adjacent to the tube wall (Figure 29-f) of an adiabatic reactor is analogous to the center fluid plug. Thus

$$Q_N \frac{dC_N}{dz} = - a(N,N-1)\ C_N[De\ k(t_{N-1})]^{0.5} \tag{71}$$

$$\rho C_p Q_N \frac{dT_N}{dz} = hp\ a(N,N-1)[t_{N-1}-T_N] \tag{72}$$

where the solid temperature is obtained via equation (56) at each numerical integration step.

In a wall-cooled reactor, equation (72) must also include a wall film heat transfer resistance:

$$\rho C_p \frac{dT_N}{dz} = hp\ a(N,N-1)[t_{N-1}-T_N] - hw\ \pi\ Dt[T_N-Twall] \tag{73}$$

The solid temperature is again obtained via equation (56).

Condensation of Equations and Solution Technique

The solution technique here is analogous to the procedure outlined earlier for heat dispersion. Description of the complete concentration and temperature profiles at any given z within an A-half-cell requires solid plug equations (56) (j=3,5,...,N-1) and (63), fluid plug equations (57) and (58) (j=2,4,...,N-2), (71) and (72) for adiabatic reactors or (73) for wall-cooled reactors. (In this section, N=Nrad, or the total number of plugs in any half-cell.) Solid plug equations (56) (j=2,4,...,N-2), and (66) for adiabatic reactors or (70) for wall-cooled reactors, fluid plug equations (57) and (58) (j=3,4,...,N-1), (64), and (65) are required for a B-half-cell. Since both temperature and concentration vary with z, each fluid plug equation must be integrated numerically from plug inlet to outlet, with solid temperatures calculated at each step. Only then can mixing calculations be made. The cells and plugs must be sized and the flows subdivided according to ε_{bed} and Dt/dp as outlined in the mass dispersion chapter. The heat transfer areas and film coefficients, hp and hw, must be determined as outlined in the heat

dispersion chapter. Then, given all necessary kinetic (rate) data (e.g., rate constant, heat of reaction, effective pellet diffusivity), the radial profiles can be obtained via the procedure below. (The following outlines a wall-cooled reactor; for an adiabatic reactor, substitute equation (66) for (70) and (72) for (73).)

1. set all inlet temperatures (solid and fluid) to Tin and all inlet concentrations to Cin;
2. within the A-half-cell, numerically integrate equations (57) and (58) (j=2,4,...,N-2), (71) and (73). At each integration step, obtain new solid temperatures via equations (56) (j=3,5,...,N-1) and (63). The outlet fluid temperatures (T_2, T_4,...,T_N) and concentrations (C_2,C_4,...,C_N) become elements of the (N/2)-long vectors $\underline{TA}$(out,n) and $\underline{CA}$(out,n), respectively, where n is the current cell number;
3. calculate B-half-cell inlet temperatures and concentrations from the previously-defined mixing matrix, $\underline{\underline{R}}$ via

$$\underline{TB}(in,n) = \underline{\underline{R}}\ \underline{TA}(out,n)$$
$$\underline{CB}(in,n) = \underline{\underline{R}}\ \underline{CA}(out,n) \qquad (74)$$

where

$$\underline{TB}(in,n)^T = [T_1\ T_3 \cdots T_{N-1}]_n$$

$$\underline{CB}(in,n)^T = [C_1\ C_3 \cdots C_{N-1}]_n$$

4. integrate equations (57) and (58) (j=3,5,...,N-1), (64) and (65) from B-half-cell inlet to outlet, calculating new solid temperatures at each integration step from equations

(56) (j=2,4,...,N-2) and (70). The outlet fluid temperatures (T_1, T_3,...,T_{N-1}) and concentrations (C_1, C_3,...,C_{N-1}) become the elements of the (N/2)-long vectors $\underline{TB}$(out,n) and $\underline{CB}$(out,n), respectively;

5. calculate the next A-half-cell inlet temperatures and concentrations from the previously-defined mixing matrix, $\underline{\underline{S}}$ via:

$$\underline{TA}(in,n+1) = \underline{\underline{S}}\ \underline{TB}(out,n)$$

$$\underline{CA}(in,n+1) = \underline{\underline{S}}\ \underline{CB}(out,n) \qquad (75)$$

where

$$\underline{TA}(in,n+1)^T = [T_2\ T_4\ \cdots\ T_N]_{n+1}$$

$$\underline{CA}(in,n+1)^T = [C_2\ C_4\ \cdots\ C_N]_{n+1}$$

6. repeat steps 2-5 until the desired number of axial cells has been traversed.

Model Parameters

The only parameters added to describe this combined case of heat and mass dispersion relate directly to the reaction involved and not to the AFM itself. These reaction-diffusion parameters (De, k, r_c, ($-\Delta H$)) must be determined independently as described elsewhere (e.g., Carberry, 1976; Froment and Bischoff, 1979; Lee, 1985; Smith, 1981). Thus, the AFM parameters are completely defined by considering only simple heat and mass dispersion characteristics.

Example Problems

Since this section must compare the AFM and the Fickian analogy for a reacting system, the appropriate Fickian equations are first presented. Then, the results of both models for several cases are compared.

The Fickian analogy equations, excluding axial dispersion, for cases involving heterogeneous or catalytic reaction (e.g., Carberry, 1976), are:

$$U_{int}\frac{\partial c}{\partial z} - Dr\left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r}\right) = -R_G\left(\frac{1-\epsilon_{bed}}{\epsilon_{bed}}\right)$$

$$U_{int}\frac{\partial T}{\partial z} - \lambda r\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right) = \left[\frac{(-\Delta H)}{\rho C_p}\right] R_G\left(\frac{1-\epsilon_{bed}}{\epsilon_{bed}}\right) \qquad (76)$$

with

$z=0$: (all r) $c=Cin$, $T=Tin$

$z>0$: $(r>0)\ \frac{\partial c}{\partial r} = \frac{\partial T}{\partial r} = 0$

$(r=Rtube)\ \frac{\partial c}{\partial r} = 0$

$-\lambda r \frac{\partial T}{\partial r} = 0$, adiabatic

$hw(T - Twall)$, wall-cooled

where

$$R_G = (Sp/Vp)C[De\ k(t_{solid})]^{0.5} \qquad (77)$$

$$(-\Delta H)R_G = hp\ (Sp/Vp)[t_{solid} - T_{fluid}] \qquad (78)$$

Here, all terms are in a consistent set of dimensions (e.g., CGS, MKS, etc.) as non-dimensionalizing these equations complicates their

numerical solution. The implicit Crank-Nicholson method (e.g., Hornbeck, 1975; Lee, 1985) was used to solve the above equations.

Figures 30 - 36 compare the AFM to Fickian analogy results for the system defined in Table 10. Bulk-averaged values for the Fickian model were determined by

$$P_{bulk} = 2\int_0^{R_{tube}} r\ P(r)dr/(R_{tube})^2 \qquad (79)$$

and for the AFM by

$$P_{bulk} = \sum_j Q_j P_j / Qtot \qquad (80)$$

where P is the property (concentration or temperature) and j corresponds to fluid plugs only (j=2, 4,. . .,N for A-half-cells and j=1,3,. . .,N-1 for B-half-cells).

Figures 30 and 31 indicate that the AFM predicts lower conversion and bluk fluid temperature than the Fickian analogy for an adiabatic reactor with a 0.5 second residence time. For a wall-cooled reactor with a 1.0 second residence time (Figures 32 and 33), the AFM conversion trend initially follows the Fickian analogy but then levels off at a lower value. Note that the reaction continues although the bulk fluid temperature remains quite low. For these first two cases neither model predicts steep radial temperature gradients. The Fickian analogy indicates a flat profile with about a 10 K drop at the wall. The AFM gives roughly the same overall temperature drop but indicates more of a profile within the bed itself.

Table 10

Example Reaction Case Parameters

$r_c = kC$ mol/cm^{3}cat-s

$k = 4.58 \times 10^8 \exp(-12000/T)\ s^{-1}$

$(-\Delta H) = 240$ kcal/mol

$\rho = 9.47 \times 10^{-4}$ g/cm^3

$C_p = 0.25$cal/g-K

$Q = 818$ cm^3/s

$De = 0.001$ cm^2/s

$dp = 0.6$cm

$Dt = 3.6$cm

$\varepsilon_{bed} = 0.40$

$Re_p = 234$

$Pr = 0.75$

$T_{in} = 600$K

$\phi in = 3.07$

Fickian parameters

$\lambda = .00152$ cal/s-cm-K

$Dr = 3.5$cm^2/s
(from Smith, 1981)

$hw = .0025$ cal/s-cm^2-K
(from Yagi and Wakao, 1959)

$hp = .0026$ cal/s-cm^2-K
(from Schlunder, 1978)

$v = 200.9$cm/s (interstitial)

Table 10-continued

AFM parameters

hw = .002 cal/s-cm^2-K

hp = .002 cal/s-cm^2-K

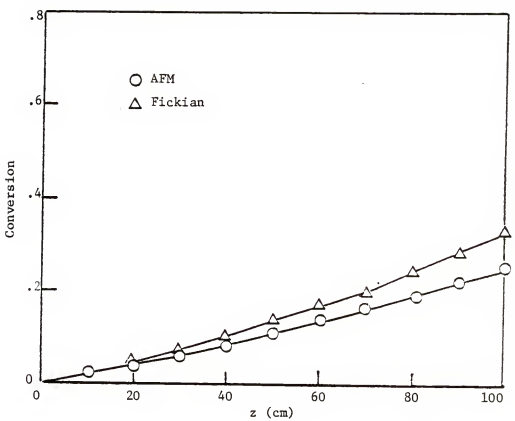


Figure 30: Conversion Profiles for Adiabatic Reactor, $C_{in}=2\times10^{-7}$, $T_{in}=600°K$

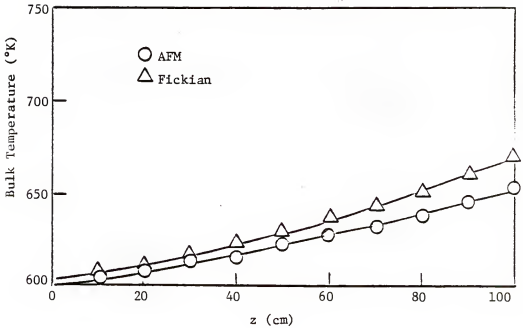


Figure 31: Bulk Temperature Profiles for Adiabatic Reactor, $C_{in}=2x10^{-7}$, $T_{in}=600°K$

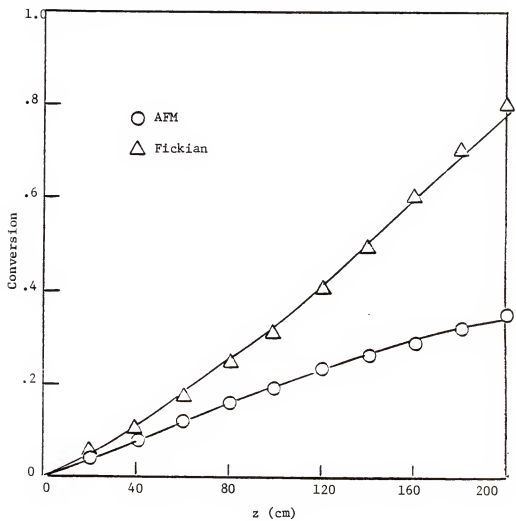


Figure 32: Conversion Profiles for Wall-cooled Reactor, $C_{in}=2x10^{-7}$, $T_{in}=Twall=600°K$

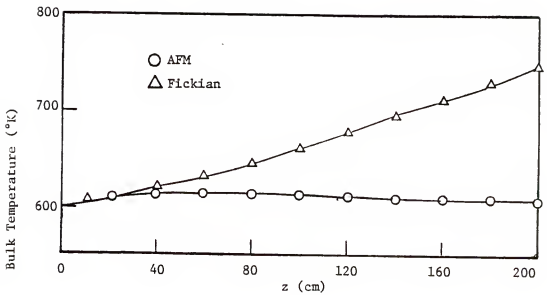


Figure 33: Bulk Temperature Profiles for Wall-cooled Reactor, $C_{in}=2x10^{-7}$, $T_{in}=Twall=600°K$

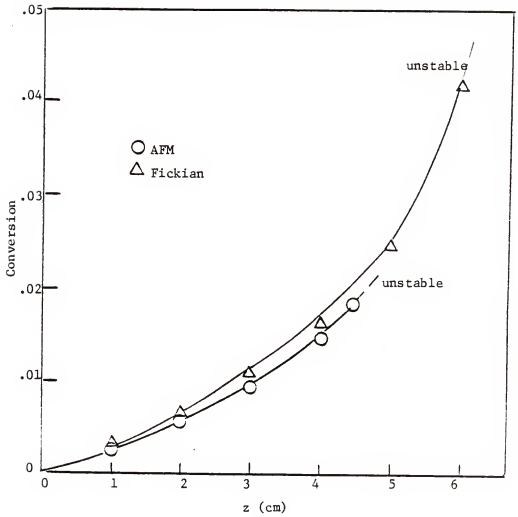


Figure 34: Conversion Profiles for Wall-cooled Reactor, Severe Inlet Conditions, $C_{in}=3x10^{-6}$, T_{in}=Twall=600°K, (at 4cm, Bulk Temperatures: AFM=639°K, Fickain=646°K)

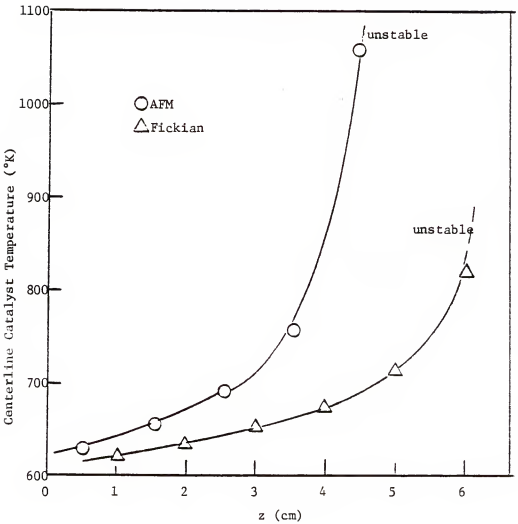


Figure 35: Centerline Catalyst Temperature Profiles for Wall-cooled Reactor with Severe Inlet Conditions

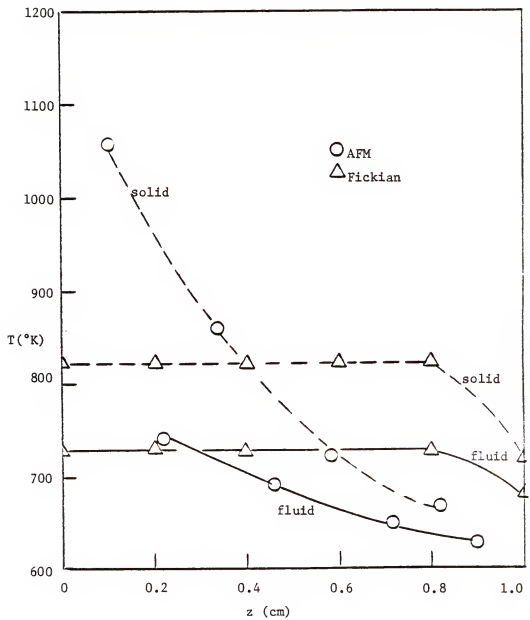


Figure 36: Radial Temperature Profiles for Wall-cooled Reactor, with Severe Inlet Conditions (at z=4.5cm for AFM, at z=6cm for Fickain Analogy)

More severe reaction conditions magnify these differences (Figures 34-36). In this case, the AFM predicts instability after only 4.5cm (0.023 sec) into the bed whereas the Fickian analogy shows the reaction to be stable until 6cm (0.03 sec) even at the low conversions predicted by both models. Although the bulk fluid temperatures at 4cm differ by only 7 K (639 K for the AFM vs. 646 K for the Fickian), the AFM indicates a much higher centerline catalyst temperature than the Fickian analogy (Figure 35). The AFM also indicates a steeper radial temperature profile and a greater difference between fluid and catalyst temperatures (Figure 36).

The AFM's distribution of flows can account for the steeper radial temperature profile. The slower flow rates near the centerline (Table 11) prolongs the residence time there thus allowing for more extent of reaction and larger temperature rise. Numerically, equations (57) and (58) support this argument since smaller Qj implies larger axial gradients. Smaller Qj, however, also implies minimal effect on bulk values (equation (80)) so that instability can be predicted even at seemingly low Tbulk. The splitting/merging at each half-cell exit eventually propogates this higher temperature radially outward.

The AFM is also more sensitive to wall conditions than the Fickian analogy. Comparison of Figure 31 (residence time of 0.5 sec) to the first 0.5 sec residnece time of Figure 33 sho that, for the less severe reaction conditions, changing from a wall-cooled (Twall=600 K) to an adiabatic reactor causes a negligible change in the Fickian predictions but a dramatic change in the AFM results. The AFM maximum-

near-wall flow distribution (Table 11) accounts for the model's sensitivity to wall conditions. Any change in the outer plugs will dominate bulk values (equation (80) and will rapidly propogate inward due to the mixing at each half-cell exit.

Figure 37 shows the effect of changing Dt/dp to 3 (Dt=3.6cm, dp=1.2cm, hp=0.0014cal/s-cm^2-K for AFM, 0.0018 cal/s-cm^2-K for Fickian) for the severe reactions of Figures 34-36. Because the increased pellet size slows the overall reaction rate, both models' predicted instabilities move farther into the reactor. However, in this case, the Fickian analogy is more conservative, i.e., it predicts the instability sooner. The AFM flow profiles (Figure 38) can explain this shift. Although the low centerline flow (Q_1 < .01 Qtot) should induce large axial concentration and temperature gradients within that plug, its effect is offset by the influence of the large wall plug flow upon mixing at the half-cell exit. (The AFM parameters in Figure 38 required ε_b=0.23 (equation (13)) to give ε_{bed}=0.40.)

Figures 39 and 40 compare the AFM and Fickian analogy for an example system which yields a Fickian-predicted hot-spot, i.e., maximum in the temperature profile. The system parameters are as given in Table 10, with a lower heat of reaction and higher wall coefficients as noted on the figures. The AFM predicts essentially no reaction after about 10cm into the vessel, whereas the Fickian analogy shows 95% conversion at 100cm. The AFM's sensitivity to wall conditions accounts for the contrast.

Table 11

AFM Flow Distribution
for Dt/dp=6, ϵ_{bed} = .40

Half-cell	Plug	Q/Qtot	u/u'
A	2	.044	1.90
	4	.159	2.28
	6	.277	2.38
	8	.520	2.67
B	1	.012	.532
	3	.093	1.33
	5	.197	1.69
	7	.697	3.57

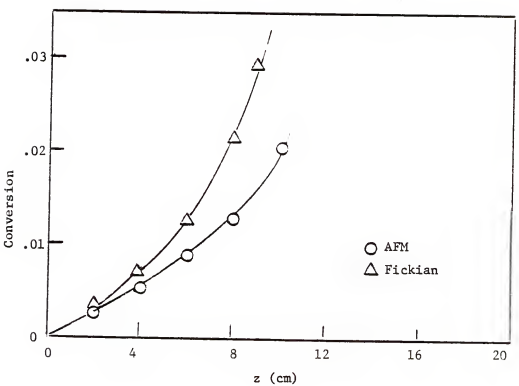
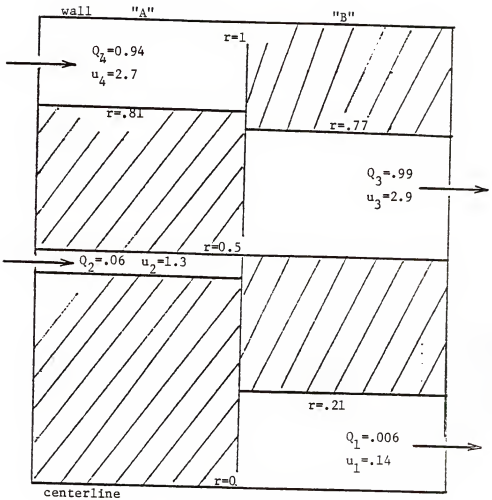


Figure 37: Conversion Profiles for Wall-cooled Reactor, Dt/dp=3.0, ϵ_{bed}= 0.40, T_{in}=Twall=600°K, C_{in}=2×10^{-7}



NOTE: Given $Q_j=Q_j/Qtot$ and $u_j=u_j/u'$

Figure 38: AFM Parameters for Dt/dp=3.0, ε_{bed}=0.40

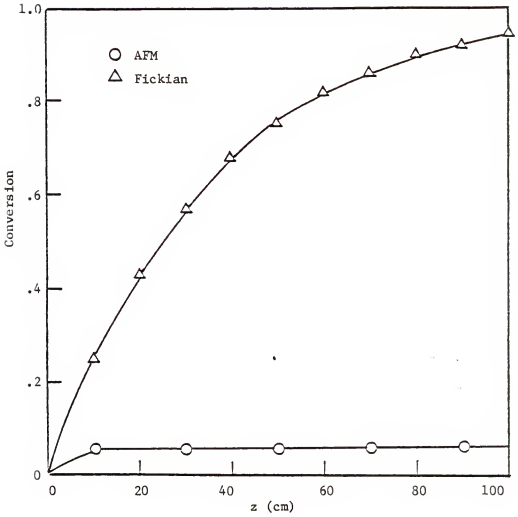


Figure 39: Conversion Profiles for Wall-cooled Reactor, Dt/dp=6.0, ϵ_{bed}=0.40, T_{in}=800°K, Twall=400°K, $C_{in}=2\times10^{-8}$, (-ΔH)=24kcal/mol, hw = 100(hw of Table 10)

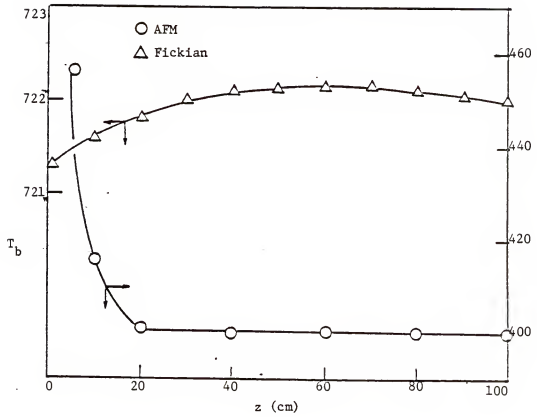


Figure 40: Temperature Profiles for Wall-cooled Reactor, Dt/dp=6.0, ϵ_{bed}=0.40, T_{in}=800°K, Twall=400°K, C_{in}=2x10^{-8}, (-ΔH)=24kcal/mol, hw=100(hw of Table 10)

Summary of AFM for Reaction

Teh Alternating Flow model views reaction in packed beds as a combination of the simple mass and heat dispersion mechanisms with reaction in the packing material, or pellets. Mass disperses axially due to bulk flow and radially because of reaction within the packing and because of mixing at each half-cell outlet. Heat disperses axially with the bulk flow, radially through pellet film resistances (to cool the heat of reaction) and from mxing at each half-cell outlet, and out at the wall through a wall film resistance. The only parameters needed for the combined, but not individual, dispersion case relate directly to reaction within the catalyst pellets and are independent of the AFM itself.

For the examples presented here, the AFM predictions differed significantly from the Fickian analogy. The AFM showed more sensitivity to wall conditions than the Fickian analogy, probably because of the AFM's maximum-near-wall flow distribution. The difference in the models' predictions fo instabilities can also be explained in terms of flow patterns.

CHAPTER V
CONCLUSIONS

The Alternating Flow Model is a viable alternative to the traditional Fickian analogy approach for modeling dispersion in packed beds. Not only does the AFM require fewer correlated parameters than the Fickian analogy, but it also meets all the dispersion model acceptability set forth in the Introduction. The AFM can also predict, solely from system geometry, the experimentally observed velocity profiles for packed beds.

The AFM equalled or surpassed the Fickian analogy in following the experimental data of the simple mass dispersion cases examined in Chapter II. For simple mass dispersion, the AFM is totally predictive: all model parameters are determined a priori from bed voidage, ε_{bed}, and relative size of tube to pellet, Dt/dp.

For most of the heat dispersion cases studied in Chapter III, the AFM followed experimental data at least as closely as the Fickian analogy. For simple heat dispersion, the AFM requires back-fitting one parameter, the wall film coefficient (hw), to each new system. The complexity of turbulent heat convection explains this need for back-fitting hw. A friction factor analogy sheds light on the observed hw vs. G^m relationship (equation (45)) and can even predict the exponent, m, for smooth tubes. The pellet film coefficient correlation

(equation (50)) can be applied to either spherical or cylindrical pellets without loss of generality. The flow rate dependence was developed from single submerged object considerations.

As a descriptor of reaction in packed beds, the AFM exhibits high sensitivity to reactor wall conditions and may predict instability (even at seemingly low bulk fluid temperatures) where the Fickian analogy does not. These differences can be explained in terms of the AFM's radial flow distribution. Thus, the AFM's ability to correctly predict packed bed velocity profiles suggests that the AFM may more closely follow reaction data. Further, the AFM's ability to predict hot spots should also be examined.

The Fickian analogy with axial dispersion predicts back-mixing where none is observed experimentally, but the AFM cannot predict the diffusion-like behavior expected in the limit of zero velocity. Thus, neither model can adequately cover all possible cases. However, the AFM should better describe cases in which ordered flow can be expected (e.g., low Dt/dp) and has the added advantage of a priori determination of all mass dispersion parameters.

The merits of the AFM discussed here warrant the further studies outlined in Appendix J.

APPENDIX A
HYDRAULIC RESISTANCES

Empty Tubes

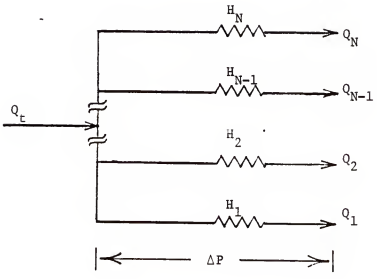
In general, the pressure drop through am empty atube can be expressed as

$$\Delta P = f\left(\frac{L}{Rh}\right)\left(\frac{Q}{A}\right)^2 / 2g_c \qquad \text{(A-1)}$$

where f is the friction factor, L is the tube length, Rh is the hydraulic radius (Rh=4 cross-sectional area/wetted perimeter), Q is the volumetric flow rate, and A is the cross-sectional area. Equation (A-1) can be rearranged to give

$$Q = a(A^2 Rh/f)^{0.5}(\Delta P)^{0.5} \qquad \text{(A-2)}$$

where a is constant. If one makes an analogy to Ohm's Law then $(\Delta P)^{0.5}$ becomes the hydraulic "voltage," $a(A^2Rh/f)^{0.5}$ the inverse of hydraulic resistance, H and Q the current flow. The total flow through a network of resistances will then subdivide according to these hydraulic resistances (Figure 41) whose form depends on pipe shape (because of Rh) and on flow regime (because of f).



$$\frac{Q_j}{Q_t} = \frac{(1/H_j)}{\sum_{j=1}^{N}(1/H_j)}$$

Figure 41: Flow Subdivision via Hydraulic Resistances

For turbulent flow, f is constant and the hydraulic resistance is given by Equation (A-4a). But, in the transition of laminar regime, f is proportional to 1/Re or Av/Q Rh so that Equation (A-2) becomes

$$Q^2 = b^2 A^2 2Rh(\Delta P)(Re)$$

or

$$Q = b\, ARh^2(\Delta P) \qquad \text{(A-3)}$$

where b is constant. The corresponding hydraulic resistance is given by Equation (A-4b).

$$A(Rh)^{0.5} \qquad \text{turbulent} \qquad \text{(A-4a)}$$

$$(1/H) =$$

$$A\, Rh^2 \qquad \text{laminar} \qquad \text{(A-4b)}$$

For tubes of circular cross-section, Rh=diameter; for empty annuli, Rh=2(outer radius - inner radius).

Packed Beds

The corresponding pressure drop relationship for packed beds includes some function of bed voidage. While the literature provides several forms of this function (e.g., Froment and Bischoff, 1979; Coulson, 1949; Ergun, 1952; Ergun and Orning; 1949; Lapin, 1962; Leva, 1947a,b) the one developed by Leva (1947b) will be used here for simplicity:

$$\Delta P = a(1-\varepsilon)U_s^2/\varepsilon^3 \qquad \text{(A-5)}$$

where a is constant and U_s is the superficial velocity based on empty tube cross-section. This can be converted to actual interstitial velocity, U_i based only on the void area, Av, as $U_s = U_i\, \varepsilon_{bed}$, where $U_i = Q/Av$. Thus, (A-5) becomes

$$\Delta P = b(1-\varepsilon)\left[\frac{Q}{A_v}\right]^2/\varepsilon \qquad \text{(A-6)}$$

so that the hydraulic resistance for a packed tube is

$$1/H = (A_v\varepsilon/(1-\varepsilon))^{0.5} \qquad \text{(A-7)}$$

and will be referred to as the "Ergun type" resistance. Note that (A-7) implies that the resistance to flow decreases as voidage increases, thus predicting the observed channelling effect of high flow at maximum voidage near the wall.

APPENDIX B
REFERENCE LIST FOR DISPERSION COEFFICIENT STUDIES

The following is a list of some works regarding axial and radial dispersion from the Fickian analogy point of view, as mentioned in the main text. No claim of completeness is made here. For complete bibliographic information, see the Bibliography.

Carberry, (1958), Chang (1982, 1983), Chung and Wen (1968), Dorweiler and Fahien (1959), Evans and Kenney (1966), Fahien and Smith (1955), Gunn (1969), Gunn and England (1971), Gunn and Pryce (1969), Klinkenberg et al. (1953), Klinkenberg and Sjeniter (1956), Kramers and Alberda (1953), Liles and Geankoplis (1960), McHenry and Wilhelm (1957), Mears (1971), Oliveros and Smith (1982), Plautz and Johnstone (1955), Roemer et al. (1962), Strang and Geankoplis (1958), Suzuki and Smith (1970), Wolff et al. (1979), Awasthi and Vasudeva (1983), Cairns and Prausnitz (1960), Carberry and Bretton (1958), Danckwerts (1953), Ebach and White (1958), Edwards and Richardson (1968), Grabmuller and Schadlich (1983), Hibilaro (1979), Hsiang and Haynes (1977), Jacques and Vermeulen (1957), Liles (1959), Miller and King (1966), Turner (1971, 1983).

APPENDIX C
AXIAL VOIDAGE VARIATION DETERMINATION

If the packed bed is considered to be a perfect cylinder filled with uniformly sized perfect spheres, and the position (coordinates) of each sphere within the cylinder is known then void fractions can be theoretically calculated. If such information is unavailable, the void fraction must be measured experimentally. Each technique is discussed below.

Experimental Measurement

Consider a cylinder marked off in equal increments along its height. Let Vol be the volume of liquid required to raise the level from one height, z1, to the next, z2, when the cylinder is empty and v be the amount of liquid required to raise the level from z1 to z2 when the cylinder is packed with pellets. Then, v is the void volume between z1 and z2 and v/Vol is the average void fraction between z1 and z2, as indicated by the dashed step-wise plot in Figure 4.

Experiments leading to Figure 4 were carried out with glass spheres (dp=1.56cm) in a 1000ml beaker (Dt=10.3cm) whose 25ml increments were 0.3cm apart. This yields Dt/dp=6.6 with axial markings every dp/5 units. Since axial voidage frequencies on the order of

less than one dp are desired, this axial increment must be small enough to achieve the desired sensitivity. Pellet diameter, dp, was determined by measuring the volume of water displaced by a set number of spheres and then calculating dp via the formula for spherical volume. The tube diameter, Dt, was calculated from the formula for cylindrical volume (volume=25ml, length= 0.3cm). The beaker was packed in several steps of pouring in a few spheres and shaking the beaker to attain the densest packing arrangement. Incremental void volumes were measured by introducing water into the packed beaker from a buret.

Theoretical Calculation

Consider a cylindrical coordinate system with its origin at the center of the lowest plane of a vertical cylinder, or tube, which is packed with uniformly sized spheres, or pellets. The tube is bounded within this coordinate system by

$$0 < z < \text{height of cylinder}$$
$$0 < r < Dt/2 \qquad \text{(C-1)}$$
$$0 < \theta < 2\pi$$

The position of each sphere within the tube is then defined by the location of its center (r_i, θ_i, z_i) and each sphere occupies the space radiating outward from its center (dp/2) in all directions. The voidage at any given axial position, z, can be determined by examining the cross-section obtained by cutting the system with a horizontal plane at that z. This would yield a circle of diameter Dt which

surrounds several smaller circles with diameters ranging from 0+ to dp/2 as shown in Figure 42. The unshaded area within the large circle represents the void area, Av. Mathematically, the void volume is given by (Av)dz and the average void volume between two axial positions z1 and z2 is found by integrating (Av)dz from z1 to z2.

Care must be taken at each axial position to include all spheres in the system which may be cut by such a plane. This is accomplished by including all spheres whose centers are not more than (dp/2) units away from the plane of interest, i.e., $\Delta z = |z_i - z| < dp/2$. Figure 43 illustrates this point. The area cut out of each eligible sphere by the plane in question is given by

$$A_i = \pi b_i^2 \qquad \text{(C-2)}$$

where

$$b_i^2 = dp^2/4 - (\Delta z)^2 \qquad \text{(C-3)}$$

The void fraction at this point is then

$$Zv/Atube = 1 - 4\Sigma A_i/Dt^2 \qquad \text{(C-4)}$$

As an example, consider the case of Dt/dp=3. The calculated void fractions for Dt/dp were given in Figure 5. Earlier, this case was described as having several layers each containing seven spheres (one at the center and six tangent to the tube wall). These layers were said to build up with the center spheres stacked and successive outer rings rotated 30 degrees. Within our system, this translates to the coordinates shown in Table 12. Figure 44 corresponds to the horizontal plane z=dp/2 while Figure 45 corresponds to the plane at z=1.5dp.

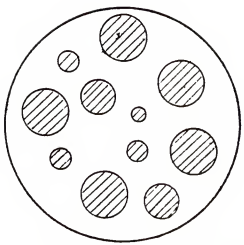
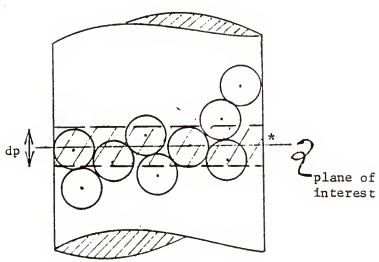


Figure 42: Horizontal Plane through Packed Tube



· pellet center

* include only those pellets whose centers fall within shaded region

Figure 43 : Inclusion of Spheres for Axial Voidage Calculations

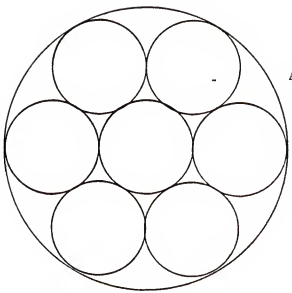


Figure 44: Horizontal Plane at z=dp/2 for Dt/dp=3

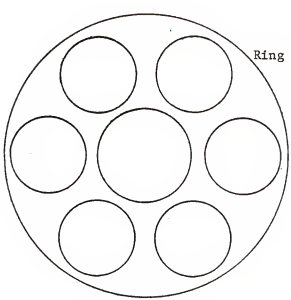


Figure 45 : Horizontal Plane at z=1.5dp for Dt/dp=3

APPENDIX D
REFERENCE LIST FOR VOID FRACTION STUDIES

Following is a list of void fraction and pellet packing study references as mentioned in the main text.

Benenati and Brosilow (1962), Bennett (1979), Cohen and Metzner (1981), Dodds (1980), Fedors (1979), Galloway et al. (1957), Hirai (1954), Haughey and Beveridge (1966), Leva and Grummer (1947b), LeGoff et al. (1985), Ouichiyama and Tanaka (1981, 1984), Pillai (1977), Ridgway and Tarbuck (1968), Roblee et al. (1958), Sloane (1984), Standish and McGregor (1978), Stanek and Eckert (1979), Wieckowski and Strek (1966).

APPENDIX E
TRANSIENT SIMULATION TECHNIQUE

The AFM prediction radial concentration profiles at any given time and axial position can be represented in the Laplace domain in equation (12) given in the main text. The motivation for such a matrix formulation was conciseness. However, the AFM transient cases were actually simulated in the time domain plug by plug and cell by cell to properly account for the radial and axial distribution of delay times. In concept, the simulation technique is straightforward, but it does require some careful "bookkeeping" at the actual computer programming stage.

The general procedure below outlines the real-time simulation of an "F-curve" experiment. All time units are assumed to be non-dimensionalized in terms of bed hold-ups. The steps are as follows:

1. Determine size and distribution of radial plugs, number of axial cells, flow distribution, and split/merge matrices ($\underline{\underline{R}}$ and $\underline{\underline{S}}$, equation (12)) as for the steady-state case.
2. After choosing Δt, subdivide each plug into elements as discussed below.
3. Set time=0.
4. Initialize concentration profile by setting all elements inside the bed at C=0.

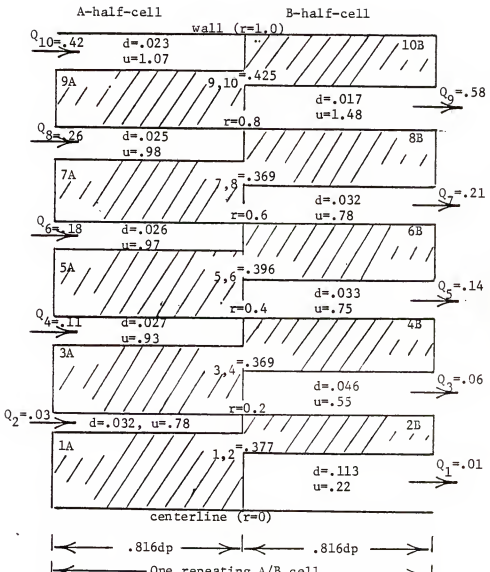
5. Let time = time + Δt.
6. Set the "bottom" (or inlet) elements of the plugs in the first half-cell at C=1. (Any convenient number may be used since the calculation of F(t) is independent of this value).
7. Determine concentration is outlet elements of all plugs as discussed below.
8. Determine concentration to be deposited in inlet elements of all plugs by the split/merge calculations, i.e.

$$\underline{B}_{in} = \underline{\underline{R}}\underline{A}_{out} \text{ or } \underline{A}_{in} = \underline{\underline{S}}\underline{B}_{out}$$

9. Determine value of F(time) as $\Sigma C_j(Qj/Qt)$ over all j in the outlet elements of the void plugs in the last half-cell (j= 2,4,6,...for A-half-cell or j=1,3,5,...for B-half-cell).
10. Repeat steps 5 through 8 until desired time has elapsed.

Consider as an example the case Dt/dp=8, z/dp=32 and ϵ_{bed}=0.39 (Jacques and Vermeulen, 1957) which gives Nz=32/1.632=19.6 or 20 (A/B) cells with each half-cell containing 5 void-full regions radially distributed as shown in Figure 46 (If (z/dp)/1.632 were, say, 19.2, the AFM would require 39 half-cells. That is, round Nz up to the nearest half.) Table 13 gives the corresponding delay times which are used to subdivide each plug into M elements where

$$M_j = d_j/\Delta t \qquad \text{(E-1)}$$



NOTE: given values are scaled by overall amounts
$Q_i = Q/Q_t$, $u_i = u/u'$, $r = r/R_{tube}$

Figure 46: Radius, Flow, and Velocity Distribution, Dt/dp=8.0, overall bed voidage = 0.39

for j=1,2,3,...,Nrad. (The time interval, Δt, is analogous to the step-size one would use with the Euler or Runge-Kutta integration techniques and should be small enough to produce significantly different Mj's.)

Since each plug consists of a certain number of time elements, the outlet concentration from the j-th plug "now" is what its inlet concentration was Mj time steps ago. In terms of real-time simulation, this translates into shifting elements within an Mj-long array as illustrated in Figure 47. At each time step, then, the "top" element is removed as the current outlet concentration (into C_{out}, all other elements are moved up one slot, and the current inlet concentration is put into the "bottom" element (from C_{in}). This shifting operation must be carried out at each time step for each plug. Note that if the inlet concentration to any given plug remains constant (as for the first half-cell) then all elements of the array will be the same after Mj time steps.

For the example case stated above, there are (20) (10)=200 arrays (one per plug) varying in length from 2 to 11 elements if Δt=0.01. One of the 20 repeating (A/B) cells is shown in Figure 48. Such a large time step was used for illustration purposes only. The actual value used to simulate this case was Δt= 0.00125.

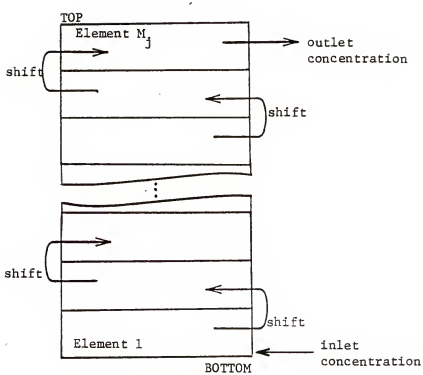
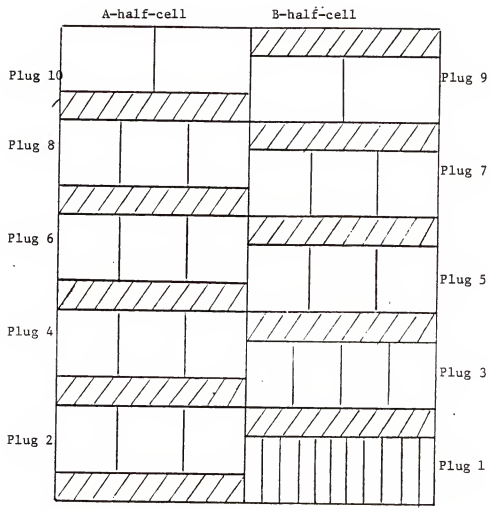


Figure 47 : Shifting Procedure for Simulation of Delay Times (Real-time)



NOTES: (a) Radial divisions not to scale
(b) Each vertical division corresponds to one time step (in void plugs)

Figure 48: Time-step Subdivision of Plugs , Dt/dp=8.0, overall bed voidage = 0.39

TABLE 13

Delay Times for Dt/dp=8, z/dp=32, ε_{bed}= 0.39

A-half-cell		B-half-cell	
plug	delay	plug	delay
2	.0321	1	.1132
4	.0270	3	.0457
6	.0259	5	.0334
8	.0254	7	.0320
10	.0234	9	.0169

Delay times calculated from equation (17).

For ease of programming, a single three-dimensional array C(I,J,K) was used to hold concentration values for all plugs, the "I" subscript defines radial plug number, "J" the axial cell number, and "K" the time step length, Mj. This array was dimensioned so that K was at least as large as the maximum Mj. Another array, NSUB(I) (I same as above), stored the Mj's so that inlet concentration values were put into C(I,J,NSUB(I)) and shifting for each plug defined by (I,J) occurred only NSUB(I) times at each real-time interval. Thus, some elements of the C(I,J,K) array were unused, but efficient storage usage was overridden by ease in programming.

APPENDIX F
COMPARISON OF AFM FLOW PROFILES BASED ON EMPTY ANNULUS AND ERGUN-TYPE HYDRAULIC RESISTANCES

The basic premise of the Alternating Flow Model (AFM) is that the bulk fluid passes through the hydraulic resistances presented by a number of (A/B) cells each consisting of a set pattern of void-full annular regions (Figure 2, main text). The empty annulus hydraulic resistances (Appendix A) are then used to determine the radial profile. But, Ergun type resistances also indicate an increase in flow with porosity. Hence, velocity and flow profiles predicted by using both types of hydraulic resistances should be compared.

Consider the case of Dt/dp=8, ε_{bed}= 0.39 (Jacques and Vermeulen, 1957) as discussed in Appendix E. The void annuli in half-cell A are defined by the radii listed in Table 14. Equation (A-7) for the Ergun type resistance requires a void cross-sectional area, Av, and average void fraction, ε, for each plug. Av is calculated directly from the plug radii and ε is taken as the average value over the evenly spaced radii as defined by equation (15), main text; Table F.1 also shows Av and ε for each plug. Table 15 gives the corresponding velocities calculated from empty annulus and Ergun type hydraulic resistances. The only noticeable difference is in the plug 2 velocities. However, because this plug represents such a small fraction of the total throughput, this difference would not significantly affect the F-curve simulation.

TABLE 14

A-Plug Size Parameters for Dt/dp=8, $\varepsilon_{bed} = 0.39$

plug	r(in)	r(out)	Av	ε_{bed}
2	.158	.200	.015	.377
4	.340	.400	.044	.369
6	.535	.600	.074	.369
8	.733	.800	.103	.369
10	.891	1.0	.153	.425

TABLE 15

Flow and Velocity Profiles by Two Types of Resistances

	Empty annulus		Ergun type	
plug	Qi/Qt	u/u'	Qi/Qt	u/u'
2	.0301	.778	.038	.969
4	.106	.928	.109	.954
6	.183	.966	.180	.952
8	.261	.984	.252	.952
10	.421	1.07	.421	1.07

z/dp=32==>Nz=20.

APPENDIX G
FICKIAN HEAT DISPERSION PARAMETER REFERENCES

The studies listed below give values and/or correlations for Fickian heat dispersion parameters in terms of other system variables. No claim regarding completeness of a literature survey is made here. For complete bibliographic information, see the Bibliography.

Baumeister and Bennett (1958), Botterill and Denolye (1978), Bunnell et al. (1949), Calderbank and Pogorski (1957), Clement and Jorgensen (1983), Coberly and Marshall (1951), Colburn (1931), Crider and Foss (1965), Duarte et al. (1985), deWasch and Froment (1972), Froment and Bischoff (1979), Gunn and Khalid (1975), Hall and Smith (1949), Hanratty (1954), Hughmark (1972, 1980), Kunii and Smith (1960), Kunii et al. (1968), Kwong and Smith (1957), Lerou and Froment (1977), Leva (1947a), Leva and Grummer (1948), Li and Finlayson (1977), Patterson and Carberry (1983), Plautz and Johnstone (1955), Reilly (1957), Schertz and Bischoff (1969), Schlunder (1978), Schotte (1960), Scott et al. (1974), Smith (1981), Vortmeyer and Winter (1982), Wakao (1976), Wakao et al. (1979), Wakao and Kato (1968), Whitaker (1972), Yagi and Kunii (1960), Yagi and Wakao (1959), Yoshida et al. (1962).

APPENDIX H
TWO-SIDED EFFECTIVENESS FACTOR FOR GENERAL
INTRINSIC KINETICS

Consider a catalyst subjected to unequal concentrations on either face (Figure 49). Tan and Smith (1980) derived a rate expression for such unsymmetric boundary conditions (with an isothermal pellet) and first-order intrinsic kinetics. Here, their idea is extended to more general intrinsic kinetics of the form:

$$r_c = k(T)f(C) \qquad \text{(H-1)}$$

where k(T) is the rate constant (dependent on catalyst temperature) and f(C) is the dependence of rate on concentration of a key component (e.g. f(C)=C for first-order, $f(C)=C^n$ for n-th order, f(C)= KC/(1+KC) for Langmuir-type, etc.). It is assumed that f(C) can be expressed solely in terms of one key component (e.g., Lee, 1985). If the pellet (slab) is isothermal then

$$\frac{d^2C}{dz^2} = \phi^2 f(C) \qquad \text{(H-2)}$$

with

$$C=C_2 \text{ at } z=-1 \text{ and } C=C_1 \text{ at } z=+1$$

where z=x/L, ϕ is the Thiele modulus, $\phi^2=L^2k(T)/De$, L is the slab half-thickness (or Vp/Sp for other shapes) and De is the effective

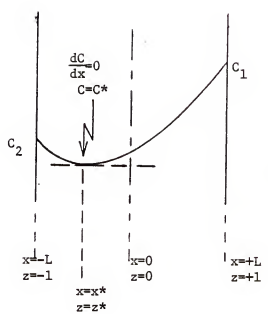


Figure 49: Catalyst Pellet (Slab) with Unsymmetric Boundary Conditions

diffusivity of the key component in the pellet. Integrating equation (H-2) from the inflection point, z*, to each face gives the concentration gradient at that face. Then, equating flux at the surface to reaction into the pellet at that face gives

$$(R_G)_i = Sp[2\ k(T)\ De \int_{C^*}^{C_i} f(C)dC]^{0.5} \qquad \text{(H-3)}$$

or

$$(R_G/Vp)_i = \frac{1}{2(Vp/Sp)} [2k(T)De \int_{C^*}^{C_i} f(C)dC]^{0.5} \qquad \text{(H-4)}$$

Note the appearance of C* (the concentration at inflection point) in these equations. For first-order kinetics, C* can be obtained directly from the analytical solution of equation (H-2) to be

$$C^* = (C_1/C_2)^{0.5}/\cosh(\phi) \qquad \text{(H-5)}$$

No analytical solution is available for more general kinetics. However, some approximations can be made. First, under certain conditions, C*-->0. Let P=C2/C1 so that $C^*=P^{0.5}C_1\cosh(\phi)$. If, for example, $0.2<P<5.0$ and $\phi_G = 3$, then $0.04<C^*/C_1<0.22$ where ϕ_G, the generalized Thiele modulus, is defined as

$$\phi_G = \frac{L(k/De)^{0.5} f(C_1)}{[2 \int_0^{C_1} f(C)dC]^{0.5}} \qquad \text{(H-6)}$$

But, such a large concentration difference (P=5) seems unlikely in AFM calculations, thus setting $C^*=0$ for $\phi_G>3$ is probably a reasonable approximation (e.g., if P=2 and $\phi_G= 3$, $C^*/C_1= 0.14$). And, as ϕ_G increases, C^* rapidly approaches zero regardless of P. Next, if these conditions are not met (i.e. ϕ_G small or P large), C^* can be approximated by substituting ϕ_G for ϕ in equation (H-5). If $\phi_G< 0.1$ the reaction is considered free of diffusion and $R_G= r_c$ (Lee, 1985).

The exact solution to equation (H-2) should be used for first-order intrinsic kinetics.

APPENDIX I
PACKING ARRANGEMENT FROM POTENTIAL ENERGY MINIMIZATION

Packed bed voidage profiles, axial and radial, can be calculated if the exact placement of each pellet within the tube is known. Experimentally, locating the exact position of each pellet would seem unnecessary since voidage profiles can be measured directly, thus overriding the need to know individual pellet locations. If, however, the packing arrangement can be determined a priori, solely from the tube and pellet sizes, there is no need to measure voidage profiles from experiments or to determine them from correlations.

Consider, then, the problem of locating N spherical pellets of diameter dp within a cylindrical tube of diameter Dt and infinite height. If the tube is filled from the top (Figure 50) each pellet will fall to the minimum possible height. The densest packing (lowest bed voidage) is attained when all pellets within the system reach their minimum height or gravitational potential. Thus, the location of each sphere within the tube can be determined by minimizing the overall system potential, Z, subject to several constraints:

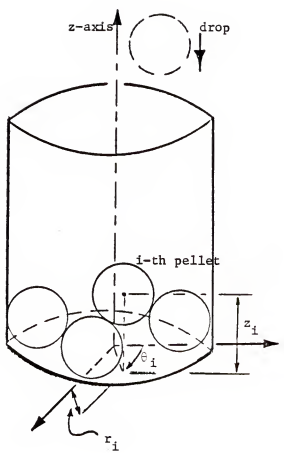


Figure 50: Spherical Pellets within Cylindrical Coordinate System

$$\text{minimize } Z = \sum_{i=1}^{N} z_i \tag{I-1}$$

$$z_i \geq dp/2 \tag{I-2}$$

$$0 \leq r_i \leq 0.5(Dt-dp) \tag{I-3}$$

$$0 \leq \theta_i \leq 2\pi \tag{I-4}$$

$$d_{i,j} \geq dp \tag{I-5}$$

(Note that the only physical parameters contained in the problem statement are tube and pellet size). Here (r_i,θ_i,z_i) locates the position of the center of the i-th sphere (in cylindrical coordinates) and $d_{i,j}$ is the distance between the centers of the i-th and j-th spheres (Figure 50). The restrictions (I-2) and (I-3) imply that each pellet can neither fall below the bottom of the tube nor extend past the tube wall, while (I-5) prevents pellets from overlapping. Constraint (I-4) defines the angular coordinate range. Note that the only nonlinearity appears in constraint (I-5) since:

$$d_{i,j}^2 = r_i^2 + r_j^2 - 2r_ir_j\cos(\theta_i - \theta_j) + (z_i - z_i)^2 \tag{I-6}$$

And, while there are only N restrictions of types (I-2) through (I-4), there are N(N-1)/2 of type (I-5). Thus, the problem is to minimize a linear objective function (I-1) of 3N variables N times

(r_i, θ_i, z_i) with 3N linear and N(N-1)/2 nonlinear constraints. While the constraints could be handled using Lagrangian multipliers and slack (Beveridge and Schechter, 1970) the resulting system would contain a prohibitive number of equations and unknowns. However, the problem can be simplified by modifying the objective function.

Consider the objective function

$$J = \sum_{i=1}^{N} z_i + \sum_{i=2}^{N} \sum_{j=1}^{i-1} f(d_{i,j}) \tag{I-7a}$$

where

$$f(d_{i,j}) = \begin{cases} 0, & d_{i,j} > dp \qquad \text{(I-7b)} \\ A(dp - d_{i,j})^{0.5}, & d_{i,j} < dp \qquad \text{(I-7c)} \end{cases}$$

and A is some known (positive) constant. The effect of the double summation is to increase the objective function for packing arrangements which cause pellets to overlap. Although a simple constant (instead of equation (I-7c)) would affect elimination of an overlap situation, the square-root functionality will allow a numerical search to differentiate "bad" from "worse". Restrictions (I-2)-(I-4) still apply.

Hence, the problem has been converted to minimization of a nonlinear objective function (equations (I-7)) of 3N variables subject to 3N linear constraints (equations (I-2)-(I-4)). The problem can be

further simplified by fixing the position of one sphere (e.g. at (0, 0,0.5dp) since only relative positions are needed. The limits of the summations of equation (I-7) would remain the same, but the number of unknowns and restrictions would each be reduced by 3 (one less each equations (I-2)-(I-4).

Once the system of equations has been solved (i.e., all pellets located), bed voidage profiles can be calculated. At any axial position, z, the average voidage over the entire tube cross-section AT THAT z is

$$\varepsilon(z) = 1 - 4 \sum_{j=1}^{N} b_j^2/D_t^2 \qquad \text{(I-8)}$$

where

$$b_j = \begin{cases} 0 & \text{if } |z_i - z| \geq dp/2 \\ [0.25dp^2 - (z_i - z)^2]^{0.5} & \text{if } |z_i - z| \leq dp/2 \end{cases} \qquad \text{(I-9)}$$

Around any cylindrical shell of radius r the average voidage over the increment $z_1 - z_2$ is

$$\varepsilon(r) = 1 - \int_{z_1}^{z_2} \left(\sum_{i=1}^{N} \alpha_i \right) dz/2\pi \qquad \text{(I-10)}$$

where

$$\alpha_i = \begin{cases} 0 & , \text{ if } |r_i - r| \geq dp/2 \\ \arccos \dfrac{r_i^2 - r^2 - (dp^2/4)}{2rr_i} & , \text{ if } |r_i - r| < dr/2 \end{cases} \qquad \text{(I-11)}$$

The integration of equation (I-11) must be numerical.

For a system with Dt/dp=1.5 the relative positions of the spheres can be intuitively determined as shown in Figure 51. If the above minimization theory holds, then solution to the corresponding set of equations should yield the desired arrangement.

The minimization technique of Luus and Jaakola (1973) was applied to a system of two pellets with Dt/dp=1.5. With one pellet fixed at (0,0,0.5dp) and an initial guess on the second pellet's position at $(0.25\pm0.125)dp,\ \pi+\pi,(1.5\pm1.0)dp$ their method gave $(r,\theta,z)_2 =$ (0.25dp, 0.994π, 1.366dp). The minimization technique of Luus and Jaakola worked equally well for other initial guesses and for two pellets with Dt/dp=2.0. But, the technique failed for more complex systems (e.g., Dt/dp=3.0 with 7 spheres, one fixed, and hence 18 unknowns). A FORTRAN program for two pellets follows.

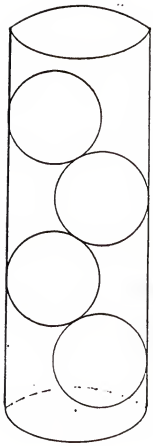


Figure 51: Stacked Arrangement of Spherical Pellets, Dt/dp=1.5

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```
C   THIS PGM FINDS THE MOST DENSE SPHERICAL PELLET PACKING                  KKP00010
C   CONFIGURATION BY MINIMIZING THE POTENTIAL ENERGY OF THE                 KKP00020
C   SYSTEM.  THAT IS, MINIMIZE THE SUM OF THE HEIGHTS OF                    KKP00030
C   THE PELLETS, GIVEN THE VARIOUS CONSTRAINTS.                             KKP00040
C                                                                           KKP00050
C   DIMENSION VARIABLES                                                     KKP00060
      DIMENSION W(6),R(6),Z(6)                                              KKP00070
      COMMON /AA/ X(6),IMAX                                                 KKP00080
      IMAX = 6                                                              KKP00090
C   VARIABLE LIST.                                                          KKP00100
C   W-ARRAY--EACH TRIPLET (W(1),W(2),W(3)) REPRESENTS THE                   KKP00110
C            R,THETA,Z (RESPECTIVELY) POSITION OF A GIVEN SPHERE            KKP00120
C            W IS THE BEST POINT FROM LAST = START PT. FOR THIS RANGE ITER. KKP00130
C   X-ARRAY--SAME SET-UP AS W-ARRAY; THESE ARE THE TEST VALUES              KKP00140
C   Z-ARRAY--SAME SET-UP AS W-ARRAY; THESE RETAIN THE BEST                  KKP00150
C            VALUES AT ANY GIVEN TRIAL WITHIN A GIVEN RANGE ITERATION       KKP00160
C   R-ARRAY--RANGES FOR CORRESPONDING W VALUES                              KKP00170
C                                                                           KKP00180
C   TUBE AND PELLET SIZE DATA                                               KKP00190
      DP = 1.0                                                              KKP00200
      DTDP = 2.                                                             KKP00210
      PI = 3.1415926                                                        KKP00220
C   INITIAL GUESS AT POSITION OF SPHERES                                    KKP00230
      W(1) = 0.5*DP                                                         KKP00240
      W(2) = 0                                                              KKP00250
      W(3) = DP/2.                                                          KKP00260
      W(4) = 0.25*DP                                                        KKP00270
      W(5) = PI                                                             KKP00280
      W(6) = 1.5*DP                                                         KKP00290
C   INITIAL RANGES                                                          KKP00300
      R(1) = 0                                                              KKP00310
      R(2) = 0                                                              KKP00320
      R(3) = 0                                                              KKP00330
      R(4) = 0.25*DP*(DTDP-1.)                                              KKP00340
      R(5) = PI                                                             KKP00350
      R(6) = DP                                                             KKP00360
C   INITIALIZE OPTIMIZATION PARAMETERS                                      KKP00370
C   JU==>NO. OF TIMES TO REDUCE RANGE SIZE                                  KKP00380
C   KP==>NO. OF POINTS TO TRY WITHIN EACH RANGE ITERATION                   KKP00390
C   E ==>AMOUNT BY WHICH TO REDUCE RANGE IN SUBSEQUENT ITERATIONS           KKP00400
9     READ(5,1000)JU,KP,E                                                   KKP00410
      IF(JU .LT. 1)GOTO 5000                                                KKP00420
      WRITE(6,2040)JU,KP,E                                                  KKP00430
C   SEED RANDOM NO. GENERATOR                                               KKP00440
      CALL RSEED(0)                                                         KKP00450
C   WRITE HEADINGS AND INITIAL GUESS                                        KKP00460
      N = IMAX/3                                                            KKP00470
      WRITE(6,2000)N                                                        KKP00480
      WRITE(6,2010)                                                         KKP00490
      WRITE(6,2020)(W(I),I=1,IMAX)                                          KKP00500
C   CALC FUNCTION AT INITIAL GUESS                                          KKP00510
      DO 5 I=1,IMAX                                                         KKP00520
5     X(I) = W(I)                                                           KKP00530
      CALL FUN(F0)                                                          KKP00540
C   WRITE FUNCTION AT INITIAL GUESS                                         KKP00550
      WRITE(6,2030)F0                                                       KKP00560
C   NOW, CALCULATION AND COMPARISON                                         KKP00570
      DO 300 J=1,JU                                                         KKP00580
      DO 400 K=1,KP                                                         KKP00590
C   PICK TRIAL POINT VIA RANDOM POSITION WITHIN PARAM. RANGES               KKP00600
      DO 300 I=1,IMAX                                                       KKP00610
      V = RNDMF(1.0)                                                        KKP00620
      V = V-0.5                                                             KKP00630
300   X(I) = W(I) + V*R(I)                                                  KKP00640
C   CHECK INEQUALITY CONSTRAINTS--ELIMINATE POINT IF DOESN'T WORK.          KKP00650
      DO 310 I=1,IMAX,3                                                     KKP00660
C   MAX RADIAL POSITION IS (DT-DP)/2...                                     KKP00670
      TEST = DP*(DTDP-1.)/2                                                 KKP00680
      IF(X(I) .LT. 0)GOTO 400                                               KKP00690
      IF(X(I) .GT. TEST)GOTO 400                                            KKP00700
C   THETA SHOULD BE BETWEEN +/- PI...                                       KKP00710
      II = I+1                                                              KKP00720
      IF(X(II) .LT. 0.0)GOTO 400                                            KKP00730
      IF(X(II) .GT. 2.0*PI)GOTO 400                                         KKP00740
C   MIN Z POSITION IS DP/2...                                               KKP00750
      II = I+2                                                              KKP00760
      IF(X(II) .LT. DP/2. ) GOTO 400                                        KKP00770
310   CONTINUE                                                              KKP00780
C   CHECK DISTANCE BETWEEN PELLET CENTERS (CANNOT BE CLOSER THAN TOUCHING)  KKP00790
      DO 330 L=1,IMAX,3                                                     KKP00800
```

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```
      DO 320 M=1,IMAX,3                                                 KKP00810
      IF(L .EQ. M)GOTO 320                                              KKP00820
      DLM = X(L)*X(L) + X(M)*X(M)                                       KKP00830
      THETA = X(L+1)-X(M+1)                                             KKP00840
      DLM = DLM - 2.0*X(L)*X(M)*COS(THETA)                              KKP00850
      DIFF = X(L+2)-X(M+2)                                              KKP00860
      DIFF = DIFF*DIFF                                                  KKP00870
      DLM = DLM + DIFF                                                  KKP00880
      DLM = SQRT(DLM)                                                   KKP00890
      IF(DLM .LT. DP/2.0)GOTO 400                                       KKP00900
320   CONTINUE                                                          KKP00910
C   SELECTED POINT MEETS CONSTRAINTS==>EVALUATE FUNCTION                KKP00920
      CALL FUN(F)                                                       KKP00930
C   CHECK FOR MINIMUM                                                   KKP00940
      IF(F .GE. FO) GOTO 400                                            KKP00950
C   WE HAVE A NEW MIN                                                   KKP00960
      FO = F                                                            KKP00970
      DO 340 I=1,IMAX                                                   KKP00980
340   Z(I) = X(I)                                                       KKP00990
C   SKIP TO HERE IF CONSTRAINT NOT MET OR FUNCTION NOT MIN              KKP01000
400   CONTINUE                                                          KKP01010
C   SAVE BEST ONE AS STARTING POINT FOR NEXT ROUND OF RANGES            KKP01020
      DO 410 I=1,IMAX                                                   KKP01030
      W(I) = Z(I)                                                       KKP01040
C   DECREASE RANGES                                                     KKP01050
      R(I) = R(I)*(1.0-E)                                               KKP01060
410   CONTINUE                                                          KKP01070
C   GO BACK FOR ANOTHER ROUND IN THE SMALLER RANGES                     KKP01080
500   CONTINUE                                                          KKP01090
C   WE'RE FINISHED!!!                                                   KKP01100
      WRITE(6,2020)(W(I),I=1,IMAX)                                      KKP01110
      WRITE(6,2030)FO                                                   KKP01120
C                                                                       KKP01130
1000  FORMAT(I3,1X,I3,1X,F5.3)                                          KKP01140
2000  FORMAT(///,' MINIMIZATION OF POTENTIAL ENERGY BY DIRECT SEARCH',  KKP01150
     1 //,' NUMBER OF PELLETS = ',I3)                                   KKP01160
2010  FORMAT(' R',12X,'THETA',8X,'Z',/,1X,3(10('-'),3X))                KKP01170
2020  FORMAT(1X,3(E10.4,3X))                                            KKP01180
2030  FORMAT(' -----FUNCTION VALUE IS ',E10.4,//)                       KKP01190
2040  FORMAT(' OPTIMIZATION PARAM...JU=',I3,'  KP=',I3,'  EPS=',F5.3)   KKP01200
C                                                                       KKP01210
      GOTO 9                                                            KKP01220
5000  STOP                                                              KKP01230
      END                                                               KKP01240
      SUBROUTINE FUN(F)                                                 KKP01250
      COMMON /AA/ X(6),IMAX                                             KKP01260
      F = 0                                                             KKP01270
      DO 10 I=3,IMAX,3                                                  KKP01280
      F = F + X(I)                                                      KKP01290
10    CONTINUE                                                          KKP01300
      RETURN                                                            KKP01310
      END                                                               KKP01320
                                                                        KKP01330
```

APPENDIX J
SUGGESTIONS FOR FUTURE WORK

Cell Length and Plug Thickness

The AFM uses porosity profile data to determine axial cell length and radial plug distribution. These parameters alone then determine the velocity profile, flow distribution, and all mass dispersion characteristics. The porosity profiles for uniformly sized spherical pellets packed in cylindrical tubes are well-documented (as discussed in the Mass Dispersion chapter), but (as mentioned in the Heat Dispersion chapter) such details are not readily available for cylindrical pellets. Since many applications involve spheres of non-uniform size distributions or non-shperical pellets, the AFM requires the corresponding porosity profiles to adequately describe such applications. And, even for uniformly sized spheres, the Cohen-Metzner radial and HCP axial porosity profiles may not apply below some small Dt/dp. The research proposed below enables the AFM to account for the effect of pellet shape on mass dispersion.

Objectives

The specific objectives are to evaluate axial and radial porosity profiles for cylindrical tubes packed with spherical pellets:

1. uniformly sized, at low Dt/dp. Below some critical Dt/dp, the previously established profiles may not apply (e.g., for Dt/dp=1.5 the axial porosity cycle width is 0.866dp vs 0.816dp for HCP);
2. of known size distribution;

and packed with cylindrical pellets (with the added objective of identifying a simple "shape normalization" parameter, i.e., an effective diameter by which irregular shapes can be equated to spheres):

3. uniformly sized, with each pellet at a known position (similar to the Dt/dp numerical calculation case presented in the Mass Dispersion chapter); this will establish a method of calculating $\varepsilon(r,z)$ in the theoretical approach to each of the remaining objectives;
4. uniformly sized, with aspect ratio l/d=1; this provides the simplest non-spherical shape;
5. uniformly sized, with aspect l/d other than 1;
6. of known size/shape distribution.

Theoretical Approaches

The exact position of each spherical pellet within a cylindrical tube can be determined by minimizing a potential function as outlined in Appendix I. Each approach below suggests modifying the minimization problem to account for shape irregularities. In each case, the resulting overall bed voidage should be checked against experimental values (measured as below or from available literature data, e.g., Leva and Grummer, 1947b).

For the spherical cases (numbers refer to objectives, above):

1. optimization as stated in Appendix I since spheres are uniformly sized;

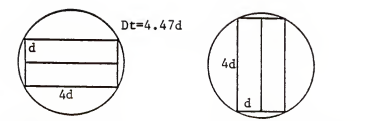
2. modify the minimization problem to include a probability that each pellet will be of certain diameter, e.g., if packing is a mixture of 30% dp_1 and 70% dp_2 then as each pellet is defined select its diameter using a normal distribution and random number. Generate a random number between -1 and +1 at each pellet definition. If the number falls within the +/-35% Gaussian limits of zero, then $dp=dp_2$. Otherwise, $dp=dp_1$. Alternatively, define pellets in groups of 10, letting three of them have $dp=dp_1$ and seven have $dp=dp_2$.

For the cylindrical pellet cases:

3. develop a procedure for specifying the position of each pellet and for calculating the corresponding $\varepsilon(r,z)$. For example, the pellet position may be defined by its centroid and its volume described by the equation for a cylindrical shell surrounding that centroid. Then, axial calculations would involve the intersection of z-planes with the individual cylinders and radial porosity would involve the intersection of a larger cylindrical shell with the individual packing cylinders. Note that, for cylindrical pellets, orientation must also be considered in defining the occupied volume, i.e., the angle between each pellet's axis and the tube axis. In

the simplest cases, all pellets would have the same orientation (e.g., pellet axes perpendicular to tube axis or pellet axes parallel to tube axis). Establish a simple test case, such as pellets with l/d=4, with two pellets per layer each in the perpendicular orientation as illustrated in Figure 52. Coordinates can be determined from geometric analysis;

4. including the orientation of each pellet increases the difficulty of the problem--orientation becomes an additional unknown. If pellet shape can be reduced via some effective diameter to a sphere, the problem is greatly simplified. Thus, attempt the minimization in the following steps:
   a. treat each pellet as a sphere with an effective diameter of ((d**2+l**2)/2)**0.5. If the overall bed voidage is close to the experimentally measured value, this is a good approximation. If not, try a different normalization (e.g., dp/4) until a good match on ε_{bed} is attained;
   b. treat each pellet as a cylinder whose position and volume are defined by the method established in objective 3; note that orientation becomes an additional unknown in the minimization problem. Start with the least complicated case of a 50/50 probability of the parallel or perpendicular orientations. Replace the $f(d_{ij})$ function (used to eliminate packing arrangements which cause two pellets to occupy the same volume) with a volume of overlap function;



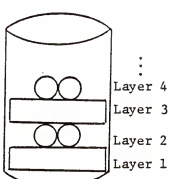


Figure 52: Predetermined Packing Geometry for Cylindrical Pellets (l/d=4)

c. include a full distribution of orientation, as opposed to the 50/50 mix. Assign orientations by random numbers within some normal distribution.

5. as for objective 4, but with size of each pellet determined from the known distribution as in objective 2;

6. as for objective 4;

Experimental Approaches

For each of the objectives listed above, the experimental technique is the same. Care should be taken to pack the tube a few pellets at a time, shaking the tube after each addition to ensure the densest packing. A screen should be placed over the top of the packed section so that pellets do not float during the measurement procedure.

1. Axial profile

a) water method--described in Appendix C. Pellets must be large enough to allow for accurate reading of the water level.

b) "wax" method--use cylindrical tubes of disposable material (e.g., commonly available containers for products such as oatmeal or cleanser). Pellets should be of material of known density that can be cut with available tools. Pack the tube as described above, secure top of packed section with screen. Fill container with hot liquid wax (slowly to avoid bubbles) or other material (e.g., epoxy or gelatin) of known density which will not contract on

hardening. Allow filling material to harden and then peel off cardboard container. Cut off ends so that remaining cylinder contains packed section only (no regions of "wax" only). Weigh the entire cylinder and measure its volume. Determine the relative amounts of "wax" and pellet material from density calculations. Cut several discs from cylinder, being sure to record their relative axial position. Each disc should be short enough to give good indication of axial periodicity, e.g., of length <dp/4. Calculate the porosity of each disc from its density (as for overall bed).

2. Radial profile--use the "wax" method, but instead of cutting discs, shave off smaller annular shells, working from outside inward. After each shaving, weigh the remaining cylindrical core to determine how much mass was lost. The density of the shaved annular shell can then be calculated as the incremental weight loss/incremental volume change. The porosity can be calculated by relating the known densities of the pellet and "wax" materials to be density of that shell.

Packed Section Velocity Profiles

Some question remains as to whether the available velocity profile data truly represent flow within the interstices of the packed section since measurements were taken in the empty tube some distance

beyond the bed exit. The most detailed data are given by Mariovoet et al. (1974) for spherical pellets at a short distance (0.625dp) into the empty tube. AFM predictions closely follow these data, but they are at only one Dt/dp value. Further, such details for cylindrical packing is unavailable. Thus, the following research is proposed to verify the AFM's method for calculating velocity profiles.

Objectives

1. verify AFM method for calculating velocity profiles for spherical and cylindrical pellets;
2. determine effect of pellet roughness on velocity profile;
3. determine range of applicability of AFM method for calculating velocity profiles.

Theoretical Approaches

Objectives 1 and 2--based on the measured (empty tubes) velocity profiles, back out what entrance profile was. Must solve Navier-Stokes (N-S) equations for empty tube. Look to work of Vortmeyer and Winter (1982) as guide; they have solved the N-S equations for set entrance velocity profiles. Or, given exact position and shape of each pellet, solve the N-S equations for velocity profiles in the packed section. (Objective 3--no definitive theoretical approach.)

Experimental Approaches

The technique of Marivoet et al. (1974) can be applied here to achieve all three objectives. Their method uses a revolving point sensor for minimum disturbance to flow pattern during measurement.

1. measure velocity profiles for wide range of Dt/dp and pellet shapes. Compare to AFM predictions;
2. compare measured velocity profiles for smooth and rough pellets of same relative size (i.e., same Dt and same dp). (Should see no difference since roughness will effect all pellets in same way);
3. measure velocity profiles over wide range of flow rates, or Re_p. Look for minimum below which and/or maximum above which the porosity-velocity relationship breaks down. Look for Dt/dp range also (e.g., for Dt/dp=1.5, the bulk fluid may "snake" through as one plug, leaving dead spaces, or regions of zero velocity, near the wall).

Applicability of AFM versus Fickian Analogy

The main text of this work shows the AFM to equal or surpass in all mass dispersion and most heat dispersion cases examined here. But, it was also pointed out that while the AFM cannot predict the diffusion-like behavior expected at very low flow rates the Fickian analogy (with axial dispersion) will predict back-mixing where none is observed experimentally. Thus, each model must have a particular range of system variables in which it should be preferred. The degree of turbulence determines whether the AFM will apply to a given situation. Turbulence in packed beds is not well-defined, however, as pointed out in the discussion of Reynolds numbers (Chapter II). The following research is therefore proposed for systems of uniformly-sized spherical packing.

Objectives

1. determine range of flow rates and fluid properties (i.e. some form of Reynolds number) over which AFM best describes dispersion in packed beds;
2. determine range of Dt/dp over which AFM best describes dispersion in packed beds (there may be a maximum above which the Fickian analogy gives satisfactory results).

Experimental Approaches

The same experiments can be used to define dispersion behavior for each of the objectives, above. The simplest experiments are those involving mass dispersion only since the pellets are inert, i.e., they act merely as barriers to flow and do not absorb any mass.

1. The steady-state injection of dye, or tracer material, at some point along the tube centerline can be used to determine the Reynolds number, Re*, at which back-mixing is observed. Experiments using salt and indicator (as described by Hiby, 1963) should be used as they give visible concentration profiles. Determine Re* for several Dt/dp values. Then, run steady-state tracer injection experiments for gases (as described by Fahien and Smith, 1955) over range of Re which includes Re*. Apparatus should be geometrically similar (i.e., same Dt/dp) to system used to determine Re*. To minimize entrance effects, the tracer injection tube should have a straight section of at least five tube diameters before entering the packed section (as opposed to "angling in" a

short distance before the packing). Verify the steady-state results with transient F-curve experiments (as described by Danckwerts, 1953) which have no entrance effects. There will probably be some minimum Re (close to Re*) below which the AFM fails to match experiment (even when the "laminar" hydraulic resistance is used to calculate flow/velocity profiles); in this range, the Fickian analogy with axial dispersion will better describe the observed concentration profiles. And, there will probably be some maximum Re above which both models can describe the observed dispersion behavior. These Re limits, however, probably depend on Dt/dp;

2. Run both steady-state and transient mass dispersion experiments for low Dt/dp. At very low Dt/dp, the injection tube must be of small size relative to the pellets so that the entrance effect will not obscure meaningful results. Alternatively, at very low Dt/dp, run only the transient experiments since the radial velocity profile determines the shape of the F-curve. There will probably be some minimum Dt/dp below which the Fickian analogy cannot match the data, regardless of Re. There will probably be some maximum Dt/dp above which both the AFM and the Fickian analogy follow the data (given the Re range determined above).

Effect of Pellet Shape on Mass Dispersion

According to the AFM, the only effect pellet shape should have on mass dispersion is via the corresponding porosity-velocity profiles. All systems compared in the Mass Dispersion chapter were for spherical pellets. It is therefore proposed here that both steady-state and transient mass dispersion experiments be carried out for systems of non-spherical pellets for which porosity profiles are known. A wide range of system variables (as described in the previous section) should be examined.

Pellet Heat Transfer Coefficient

Chapter III covered steady-state heating of a packed bed with constant wall temperature. Such cases involve both wall and pellet heat transfer characteristics and any results thus obtained may be coupled. The research proposed here eliminates wall heat transfer to verify the pellet coefficients presented earlier.

Objectives

1. verify the hp correlation (equation 50)) presented earlier for uniformly sized spherical pellets of low thermal conductivity;
2. verify the shape factor, γ (equation (50)), for cylindrical pellets and determine whether γ depends on aspect ratio of individual pellets;
3. determine effect of mixture of pellet sizes on hp;
4. determine the effect of pellet surface roughness on hp;

5. determine the effect of fluid properties on hp;
6. determine the effect of pellet material properties (e.g., thermal conductivity, specific heat, etc.) on hp;
7. verify that tube characteristics do not effect hp.

Experimental Approaches

Decoupling pellet from wall heat transfer requires an insulated tube. In this case, the simplest heat transfer experiment is analogous to the steady-state injection of tracer material: the steady-state injection of heated fluid at some point along the tube axis. To minimize entrance effects, the injection tube should be small relative to pellet size and should have a straight segment of at least five tube diameters before entering the packed section. Radial temperature profiles should be measured as close as possible to the top of the bed to minimize exit effects. Axial profiles should be obtained by successively adding more packing material (as described by Fahien and Smith, 1955) as opposed to inserting thermowells into the packed section. For each of the objectives, the following details should be observed:

1. run the point-source experiments for a "base case" system (i.e., smooth spherical pellets in smooth tube). The tube material should have a low enough thermal conductivity to be considered insulating (e.g., glass). Otherwise, there will be heat transfer to raise the wall temperature. Examine a wide range of flow rates and pellet sizes to verify the square-root correlation of hp to (G/dp);

2. run experiments as described for objective 1, using cylindrical pellets;
3. run experiments as described for objective 1 for known size distribution of spherical pellets. Determine whether some additive form of equation (50) can be used or whether new correlation must be developed for each size mixture;
4. run the experiments described for objective 1, but with uniformly sized spherical pellets of varying degrees of surface roughness, e.g., catalyst support material. The value of γ (equation (50)) may be effected by pellet roughness, which can be described--
   a) visually (qualitative);
   b) by pellet porosity (an indication of "holes" on the surface;
   c) by pressure drop relative to smooth tubes of same geometry, i.e., roughness = $(\Delta P)_{rough}/(\Delta P)_{smooth}$ at same Re and Dt/dp;
5. run experiments for objective 1 with fluids other than air (for which equation (50) was developed). Check correlation with fluid properties such as thermal conductivity, specific heat, etc.;
6. run experiments for objective 1 with materials of increasing thermal conductivity. There will be some maximum at which the

conduction between pellets assumption no longer holds. Below this maximum, however, check correlation of hp with pellet material properties such as thermal conductivity, specific heat, etc.;

7. run experiments for objective 1 with tubes of different sizes. While materials of varying degrees of surface roughness would be desirable, care should be taken in selecting low thermal conductivity (i.e., insulating) materials for the reasons stated above.

Wall Heat Transfer Coefficient

Once the pellet heat transfer coefficient has been independently verified as described above, the constant wall temperature experiments discussed earlier can be used to verify the AFM hw correlation. The same results can be used to examine the weighted average for calculating "wall solid plug" temperatures (equation (37)).

Objectives

1. verify hw correlation form;
2. determine the effect of tube characteristics (e.g., roughness, Dt, Dt/dp, thermal conductivity, heat capacity, etc.) on hw;
3. determine effect of bulk fluid properties (e.g., thermal conductivity, heat capacity, etc.) on hw;
4. verify weighted-average calculation of wall solid plug temperatures.

Theoretical Approaches

The complexity of convective film heat transfer precludes strictly theoretical prediction of hw. However, several alternatives to the "stagnant film" argument leading to the weighted-average temperature should be considered:

1. replace the stagnant film analysis with conduction from wall to solid. Note that not all of wall area would be involved in conduction because of imperfect contact between pellets and tube. The contact area would be determined empirically. This analysis would lead to some constant value for the equivalent of $a(s,w)h^*$, or a weighting that would vary with flow rate, G;
2. consider conduction (rather than convection) through the stagnant film. Film may not be strictly stagnant, so that its thickness will depend on flow rate, G. This analysis would lead to a flow-dependent equivalent of $a(s,w)h^*$, or a weighting that would remain essentially independent of flow rate. Look to boundary-layer theory as guide to determining film thickness.

Experimental Approaches

Each of the above objectives can be examined by the constant wall temperature experiments described by Yagi and Wakao (1959). Radial and axial temperature profiles and bulk outlet temperatures should be measured for each run. Radial profiles should be measured as close

as possible to the top of bed to avoid exit effects. Axial profiles should be obtained by adding packing, as opposed to inserting thermowells, to avoid disturbances to packing geometry.

3. Select a base case as described in Chapter III (e.g., smooth tube, smooth uniformly sized pellets). Run the experiments, covering a wide range of flow rates. Compare to AFM results using the independently determined hp (previous section) and the 10%-90% weighting given in Chapter III. If (log hw)-(log G) plot exhibits such scatter, either correlation form is invalid or weighting (for wall solid plug) may be function of flow rate (as described in Theoretical Approaches, above). Run for several pellet sizes;
4. run the experiments as described for objective 1, varying tube size (with constant Dt/dp), tube size (with changing Dt/dp), and tube material. Check correlation of hw with these parameters;
5. run experiments for objective 1 but with fluids other than air (for which all cases discussed in Chapter III were run). Check correlation of hw with fluid properties;
6. this objective is incorporated into the experiments for objective 1.

AFM as a Reactor Design Tool

The AFM has particular applicability to situations where ordered flow can be expected, such as low Dt/dp. Such situations are common in applications involving highly exothermic catalytic reactions where only a few pellets are placed across the tube diameter to facilitate cooling. It was shown earlier that the AFM and Fickian analogy predict different behavior for catalytic reaction within the pellets of packed beds. Thus, the following research is proposed.

Objectives

1. check the AFM's ability to match laboratory data for reaction in beds packed with spherical catalyst pellets;
2. check the AFM's ability to predict hot spots in wall-cooled reactors;
3. evaluate the AFM as a reactor design tool.

Experimental Approaches

For each of the above objectives, the deoxygenation of ethylene oxide to ethylene is proposed as the test reaction since its kinetics have been previously determined (Hong, 1984; Akella, 1983).

1. run the reaction at concentrations and flow rates that mesh with AFM assumptions (i.e., diffusion-limited, no back-mixing, etc.). First, run adiabatic reactions (if possible without instabilities) so that there is no wall heat transfer effect and some of the AFM assumptions can be verified. Next, run with constant wall temperature so that hw correlations and other related assumptions can be verified. Spherical pellets

should be used since porosity and velocity profiles are well-understood. Radial, axial, and bulk-averaged outlet profiles of concentration and temperature should be measured for each experiment. Radial profiles should be taken as close as possible to the top of the bed (to avoid exit effects) and axial profiles should be measured by successively adding packing (to avoid disturbance to packing geometry). Several values of Dt/dp should be tried to check the effect of flow distribution on conversion;

2. run the reactions as described for objective 1, but at more severe conditions and constant coolant (wall) temperature. Increase bed depth and/or vary reaction conditions until a hot spot (axial peak) in temperature is observed. Check against AFM predictions;

3. the example problems presented in Chapter IV suggest instabilities at the centerline can occur before they occur in the outer regions of the tube. This suggests that, in cases with such severe conditions, it may be advantageous to pack the bed with inert (non-reacting) pellets along the tube axis surrounded by active catalytic pellets. According to the AFM, little conversion would be lost because of the small proportion of the total fluid which flows near the bed center. If the AFM proves successful in following the reaction data described for objectives 1 and 2, above, its ability to suggest such alternatives to normal operating procedure should be exploited.

APPENDIX K
FORTRAN PROGRAM LISTINGS

Steady-state Mass Dispersion

The following program consists of a main calling routine and several subroutines. Program flow is as follows:

1. determine radial subdivisions RA(I) and RB(I) given Dt/dp and porosity about which radial cycles oscillate (EBAR) (subroutine VOID performs numerical integration of porosity function EFUNC);
2. subdivide flows (G(I) according to void cross-sectional areas A(I) and hydraulic radii RH(I) (subroutine ANN does this; two versions are included--the first version is for turbulent and the second for laminar hydraulic resistances);
3. calculate velocities;
4. determine weighting factors for mixing W(I) (subroutine MIX1);
5. initialize concentrations C(I);
6. march down reactor from inlet to outlet, transversing NLONG axial cells (NOTE: run cases with NLONG=1 for trial and error on the value of EBAR which gives the desired overall bed voidage, then run for the entire bed length to get concentration profiles).

a) A-to-B transition (subroutine MIX2 with ITRANS=0)

b) B-to-A transition (subroutine MIX2 with ITRANS=1)

Other variables and program steps are commented in the listing. All flow, area, and radius variables are scaled by total flow, total tube cross-section, and tube radius, respectively.

```
C   PROGRAM NAME 'AAPVJ FORTRAN'                                          DUM00010
C                                                                         DUM00020
C  ---------------------------------------------------                    DUM00030
C  THIS RUN FOR DATA OF LATINEN                                           DUM00040
C     4-INCH PIPE                                                         DUM00050
C  ---------------------------------------------------                    DUM00060
C                                                                         DUM00070
C   LAST UPDATE/OSE ON 14 MAY 85                                          DUM00080
        DIMENSION D(10)                                                   DUM00090
        DIMENSION Q(100),R(100),A(100),VEL(100)                           DUM00100
        DIMENSION W(100),C(100)                                           DUM00110
        DIMENSION RA(100),RB(100)                                         DUM00120
C   THIS PROGRAM CALCULATES FLOWS AND CONCENTRATIONS GIVEN                DUM00130
C   ANNULUS DIMENSIONS.                                                   DUM00140
C                                                                         DUM00150
        DATA NLONG,NPRINT /1,0/                                           DUM00160
        DATA C /100*0.0/                                                  DUM00170
        DATA NO,D /1, 12.8, 11.1, 13.3, 25.6, 6*0.0/                      DUM00180
        DATA R /100*0.0/                                                  DUM00190
        DATA FUDGE /0.05/                                                 DUM00200
C   CALC AREAS BASED ON DTDP AND EA                                       DUM00210
        DTDP = 13.2                                                       DUM00220
        DO 10 I=1,100                                                     DUM00230
10      W(I) = 20.0                                                       DUM00240
CCC     Z = DTDP + 0.5                                                    DUM00250
C   NOW, TRY ASSIGNING NO. CELLS BASED ON CORRELATION...                  DUM00260
        Z = DTDP/0.816 + 0.5                                              DUM00270
        N = Z                                                             DUM00280
        Z = N                                                             DUM00290
        Z = 0.5*Z                                                         DUM00300
        NB = Z                                                            DUM00310
        NA = N-NB                                                         DUM00320
C   RESTRICT TO EVEN NO. SEGMENTS                                         DUM00330
        IF(NA .GT. NB)NB = NA                                             DUM00340
        N = NA+NB                                                         DUM00350
        WRITE(6,2020)DTDP,N,NA,NB                                         DUM00360
C   SIZE RADII                                                            DUM00370
C   SET UP TO DO INCREASING EA'S...                                       DUM00380
C   SIZE EVENLY SPACED RADII                                              DUM00390
        ZN = N/2                                                          DUM00400
        DELR = 1.0/ZN                                                     DUM00410
        R(2) = DELR                                                       DUM00420
        DO 80 I=4,N,2                                                     DUM00430
        R(I) = R(I-2) + DELR                                              DUM00440
80      CONTINUE                                                          DUM00450
C   DETERMINE EPS FOR EACH SEGMENT...                                     DUM00460
        EHAR = 0.3600                                                     DUM00470
C   VOID FRACTION OF FIRST SEGMENT                                        DUM00480
        CALL VOID(100,DTDP,0.0,R(2),EHAR,E1)                              DUM00490
        I=2                                                               DUM00500
        WRITE(6,2010)I,E1                                                 DUM00510
100     RA(1) = (1.0-E1)*R(2)*R(2)                                        DUM00520
        RA(1) = SQRT( RA(1) )                                             DUM00530
        RB(1) = E1*R(2)*R(2)                                              DUM00540
        RB(1) = SQRT( RB(1) )                                             DUM00550
        MAX = N-1                                                         DUM00560
        DO 120 I=3,MAX,2                                                  DUM00570
C   VOID FRACTIONS OF RADIAL CELLS BASED ON CORRELATION                   DUM00580
        RHO2 = R(I+1)                                                     DUM00590
        RHO1 = R(I-1)                                                     DUM00600
        CALL VOID(100,DTDP,RHO1,RHO2,EHAR,EHAT)                          DUM00610
        IE = I+1                                                          DUM00620
        WRITE(6,2010)IE,EHAT                                              DUM00630
        XX = R(I+1)*R(I+1) - R(I-1)*R(I-1)                                DUM00640
        RA(I) = (1.0-EHAT)*XX                                             DUM00650
        RA(I) = R(I-1)*R(I-1) + RA(I)                                     DUM00660
        RA(I) = SQRT( RA(I) )                                             DUM00670
        RB(I) = EHAT * XX                                                 DUM00680
        RB(I) = R(I-1)*R(I-1) + RB(I)                                     DUM00690
        RB(I) = SQRT( RB(I) )                                             DUM00700
120     CONTINUE                                                          DUM00710
        MAX = N-1                                                         DUM00720
        WRITE(6,2150)                                                     DUM00730
        WRITE(6,2160) (RA(I),R(I+1),I=1,MAX,2)                            DUM00740
        WRITE(6,2160) (RB(I),R(I+1),I=1,MAX,2)                            DUM00750
        CALL ANN(NA,NB,Q,R,A,E1,E2,RA,RB)                                 DUM00760
        N = NA+NB                                                         DUM00770
        DO 200 I=1,N                                                      DUM00780
200     VEL(I) = E1*Q(I)/A(I)                                             DUM00790
C   WRITE RESULTS                                                         DUM00800
```

```
      WRITE(6,2050)                                                     DUM00810
      IF( NA .GT. NB)GOTO 390                                           DUM00820
      DO 300 I=2,N,2                                                    DUM00830
      J=I-1                                                             DUM00840
      WRITE(6,2060) I,A(I),Q(I),VEL(I),J,A(J),Q(J),VEL(J)               DUM00850
300   CONTINUE                                                          DUM00860
      WRITE(6,2070) E1,E2                                               DUM00870
      GOTO 410                                                          DUM00880
390   CONTINUE                                                          DUM00890
      MAX = N-1                                                         DUM00900
      DO 400 I=1,MAX,2                                                  DUM00910
      J = I+1                                                           DUM00920
      WRITE(6,2060) I,A(I),Q(I),VEL(I),J,A(J),Q(J),VEL(J)               DUM00930
400   CONTINUE                                                          DUM00940
      WRITE(6,2060) N,A(N),Q(N),VEL(N)                                  DUM00950
      WRITE(6,2070) E1,E2                                               DUM00960
410   CONTINUE                                                          DUM00970
      WRITE(6,2150)                                                     DUM00980
      WRITE(6,2160) (R(I),I=1,N)                                        DUM00990
      CALL MIX1(NA,NB,Q,N)                                              DUM01000
      WRITE(6,2170)                                                     DUM01010
      WRITE(6,2160) (R(I),I=1,N)                                        DUM01020
      IF(NA .GT. NB)C(1) = 9.1E-3/Q(1)                                  DUM01030
      IF(NA .EQ. NB)C(2) = 9.1E-3/Q(2)                                  DUM01040
      N = NA + NB                                                       DUM01050
C  NOW, CALC CONCENTRATIONS...                                          DUM01060
      WRITE(6,2230)                                                     DUM01070
      KCONT = 0                                                         DUM01080
500   KCONT = KCONT+1                                                   DUM01090
      IF(KCONT .GT. NLONG)GOTO 1000                                     DUM01100
      IF(KCONT .LT. 2) GOTO 510                                         DUM01110
      CALL MIX2(1,NA,NB,Q,N,C)                                          DUM01120
510   CALL MIX2(0,NA,NB,Q,N,C)                                          DUM01130
      IF(KCONT .LT. NPRINT)GOTO 710                                     DUM01140
      WRITE(6,2240)KCONT                                                DUM01150
      IF(NA .GT. NB) GOTO 690                                           DUM01160
C  CALC AVG CONC IN EACH HALF-CELL FOR NA=NB (==>A'S EVEN)              DUM01170
      CABAR = 0                                                         DUM01180
      CBBAR = 0                                                         DUM01190
      DO 520 I=2,N,2                                                    DUM01200
      CABAR = CABAR + C(I)*Q(I)                                         DUM01210
      CBBAR = CBBAR + C(I-1)*Q(I-1)                                     DUM01220
520   CONTINUE                                                          DUM01230
      DO 600 I=2,N,2                                                    DUM01240
      J = I-1                                                           DUM01250
      CA = C(I)/CABAR                                                   DUM01260
      CB = C(J)/CBBAR                                                   DUM01270
      WRITE(6,2250)I,C(I),CA,J,C(J),CB                                  DUM01280
600   CONTINUE                                                          DUM01290
      GOTO 710                                                          DUM01300
690   CONTINUE                                                          DUM01310
C  CALC AVG CONC IN EACH HALF-CELL FOR NA>NB (==>A'S ODD)               DUM01320
      CABAR = 0                                                         DUM01330
      CBBAR = 0                                                         DUM01340
      MAX = N-1                                                         DUM01350
      DO 695 I=2,MAX,2                                                  DUM01360
      CABAR = CABAR + C(I-1)*Q(I-1)                                     DUM01370
      CBBAR = CBBAR + C(I)*Q(I)                                         DUM01380
695   CONTINUE                                                          DUM01390
      CABAR = CABAR + C(N)*Q(N)                                         DUM01400
      MAX = N-1                                                         DUM01410
      DO 700 I=1,MAX,2                                                  DUM01420
      J = I+1                                                           DUM01430
      CA = C(I)/CABAR                                                   DUM01440
      CB = C(J)/CBBAR                                                   DUM01450
      WRITE(6,2250) I,C(I),CA,J,C(J),CB                                 DUM01460
700   CONTINUE                                                          DUM01470
      CA = C(N)/CABAR                                                   DUM01480
      WRITE(6,2250) N,C(N),CA                                           DUM01490
710   CONTINUE                                                          DUM01500
      GOTO 500                                                          DUM01510
1000  CONTINUE                                                          DUM01520
C  FORMATS...                                                           DUM01530
2010  FORMAT(' I =',I4,'  EPS = ',E11.4)                                DUM01540
2015  FORMAT(' ALPHA =',E11.4)                                          DUM01550
2020  FORMAT(' DTDP = ',E11.4,'  N =',I3,' NA =',I3,' NB =',I3)         DUM01560
2030  FORMAT(' D1/8 =',E11.4)                                           DUM01570
2040  FORMAT(' F = ',E11.4)                                             DUM01580
2050  FORMAT(20X,'A',43X,'B',//,2X,40('-'),2X,40('-'),/,                DUM01590
     1 2(2X,'I',7X,'A',11X,'F',9X,'EL  ',5X),/,                         DUM01600
```

```
     2 1X,2('---',2X,3('----------',2X))                                DUM01610
2060 FORMAT(1X,2(I3,2X,3(E10.4,2X)))                                    DUM01620
2070 FORMAT(' E1 = ',E11.4,'  E2 = ',E11.4)                             DUM01630
2150 FORMAT(' RADII...')                                                DUM01640
2160 FORMAT(5(2X,E11.4))                                                DUM01650
2170 FORMAT(' MIXING WEIGHT FACTORS. . .')                              DUM01660
2230 FORMAT(9X,'A',30X,'B',/,2(2X,29('-')),/,                           DUM01670
     1 2X,2(1X,'I',8X,'C',7X,3X,'C/CAVG',8X),/,                         DUM01680
     2 2X,2('---',2X,'----------',2X,'----------',2X))                  DUM01690
C23456789.123456789.123456789.123456789.123456789.123456789.           DUM01700
2240 FORMAT(' CELL NO ',I5)                                             DUM01710
2250 FORMAT(2X,2(I3,2X,E11.4,2X,E11.4,2X))                              DUM01720
2260 FORMAT(' BA = ',E11.4,'  EBBD = ',E11.4)                           DUM01730
2270 FORMAT(' CALC. INVALID VOID FRACT.  PGM ABORTED ')                 DUM01740
2290 FORMAT(' F =',E11.4,'  SUM =',E11.4,'  EPS1 =',E11.4)              DUM01750
     STOP                                                               DUM01760
     END                                                                DUM01770
C                                                                       DUM01780
     SUBROUTINE ANM(NA,NB,Q,R,A,E1,E2,BA,BB)                            DUM01790
     DIMENSION BA(100),BB(100)                                          DUM01800
     DIMENSION Q(100),R(100),BB(100),A(100)                             DUM01810
C  CALC  HYDRAULIC RADII, AND AREAS                                     DUM01820
     N = BA + BB                                                        DUM01830
C  A HALF-CELL                                                          DUM01840
     DO 10 I=2,N,2                                                      DUM01850
     BH(I) = B(I) - BA(I-1)                                             DUM01860
     A(I) = R(I)*B(I) - BA(I-1)*BA(I-1)                                 DUM01870
10   CONTINUE                                                           DUM01880
C  B HALF-CELL                                                          DUM01890
     BH(1) = BB(1)                                                      DUM01900
     A(1) = BB(1)*BB(1)                                                 DUM01910
     MAX = N-1                                                          DUM01920
     DO 20 I=3,MAX,2                                                    DUM01930
     BH(I) = BB(I) - B(I-1)                                             DUM01940
     A(I) = BB(I)*BB(I) - B(I-1)*B(I-1)                                 DUM01950
20   CONTINUE                                                           DUM01960
C  NOW, DETERMINE FLOWS AND POROSITIES OF A AND B SEGS                  DUM01970
C  DEPENDS ON NA AND NB                                                 DUM01980
     IF(NA .LE. NB) GOTO 500                                            DUM01990
C  THIS SECTOR FOR NA GT NB                                            DUM02000
C  FLOW DISTRIBUTION AND POROSITY                                       DUM02010
     E1 = 0.0                                                           DUM02020
     SUM = 0.0                                                          DUM02030
     DO 100 I=1,N,2                                                     DUM02040
     E1 = E1 + A(I)                                                     DUM02050
100  SUM = SUM + A(I)*SQRT(BH(I))                                       DUM02060
     DO 110 I=1,N,2                                                     DUM02070
     Q(I) = A(I)*SQRT(BB(I))/SUM                                        DUM02080
110  CONTINUE                                                           DUM02090
C  B SEGMENT                                                            DUM02100
     E2 = 0.0                                                           DUM02110
     SUM = 0.0                                                          DUM02120
     M1 = N-1                                                           DUM02130
     DO 120 I=2,M1,2                                                    DUM02140
     E2 = E2+A(I)                                                       DUM02150
120  CONTINUE                                                           DUM02160
     XX = A(N-1)*SQRT( BH(N-1) )                                        DUM02170
     YY = A(N-3)*SQRT( BH(N-3) )                                        DUM02180
     Q(N-1) = Q(N) + Q(N-2)*XX/(XX+YY)                                  DUM02190
     XX = A(2)*SQRT(BH(2))                                              DUM02200
     YY = A(4)*SQRT(BH(4))                                              DUM02210
     Q(2) = Q(1) + Q(3)*XX/(XX+YY)                                      DUM02220
     MAX = N-3                                                          DUM02230
C  DON'T NEED FOLLOWING IF N .LE. 5                                     DUM02240
     IF(N .LE. 5)GOTO 1000                                              DUM02250
     DO 130 I=4,MAX,2                                                   DUM02260
     XX = A(I)*SQRT(BH(I))                                              DUM02270
     YY = A(I-2)*SQRT(BH(I-2))                                          DUM02280
     ZZ = A(I+2)*SQRT(BH(I+2))                                          DUM02290
     Q(I) = Q(I-1)*XX/(XX+YY) + Q(I+1)*YY/(YY+ZZ)                       DUM02300
130  CONTINUE                                                           DUM02310
     GOTO 1000                                                          DUM02320
500  CONTINUE                                                           DUM02330
C  THIS SECTION FOR NA=NB                                               DUM02340
C  FLOW DISTRIBUTION AND POROSITY                                       DUM02350
C  A-SEGMENT                                                            DUM02360
     SUM = 0.0                                                          DUM02370
     E1 = 0.0                                                           DUM02380
     DO 510 I=2,N,2                                                     DUM02390
     E1 = E1 + A(I)                                                     DUM02400
```

```
      SOM = SOM + A(I)*SQRT(RR(I))                                      DOM02810
      DO 520 I=2,N,2                                                    DOM02820
      Q(I) = A(I)*SQRT(RR(I))/SOM                                       DOM02830
520   CONTINUE                                                          DOM02840
C  B-SEG                                                                DOM02850
      E2 = 0.0                                                          DOM02860
      SUM = 0.0                                                         DOM02870
      N1 = N-1                                                          DOM02880
      DO 530 I=1,N1,2                                                   DOM02890
      E2 = E2+A(I)                                                      DOM02900
530   CONTINUE                                                          DOM02910
C  THY SOMEIVIDING BASED ON SQRT(RR)                                    DOM02920
C        --INSTEAD OF A*SQRT(RR)                                        DOM02930
      XX = A(N-1)*SQRT(RR(N-1))                                         DOM02940
      YY = A(N-3)*SQRT(RR(N-3))                                         DOM02950
      Q(N-1) = Q(N) + Q(N-2)*XX/(XX+YY)                                 DOM02960
      XX = A(1)*SQRT(RR(1))                                             DOM02970
      YY = A(3)*SQRT(RR(3))                                             DOM02980
      Q(1) = Q(2)*XX/(XX+YY)                                            DOM02990
      MAX = N-3                                                         DOM03000
C  DON'T NEED FOLLOWINGIF N .LE. 4                                      DOM03010
      IF( N .LE. 4)GOTO 1000                                            DOM03020
      DO 540 I=3,MAX,2                                                  DOM03030
      XX = A(I)*SQRT(RR(I))                                             DOM03040
      YY = A(I-2)*SQRT(RR(I-2))                                         DOM03050
      ZZ = A(I+2)*SQRT(RR(I+2))                                         DOM03060
      Q(I) = Q(I-1)*XX/(XX+YY) + Q(I+1)*XX/(XX+ZZ)                      DOM03070
540   CONTINUE                                                          DOM03080
1000  RETURN                                                            DOM03090
      END                                                               DOM03100
C                                                                       DOM03110
      SOBROUTINE VOID(NDIV,DTDP,RHO1,RHO2,EBAR,EPS)                     DOM03120
      ZNDIV = NDIV                                                      DOM03130
      DELR = (RHO2 - RHO1 ) /ZNDIV                                      DOM03140
      ROLD = RHO1                                                       DOM03150
      FOLD = RHO1*EFUNC(RHO1, DTDP, EBAR)                               DOM03160
      SUM = 0.0                                                         DOM03170
      DO 100 I=1,NDIV                                                   DOM03180
      RNEW = ROLD + DELR                                                DOM03190
      FNEW = RNEW * EFUNC(RNEW, DTDP, EBAR)                             DOM03200
      FINT = 0.5*DELR*(FNEW + FOLD)                                     DOM03210
      SUM = SUM + FINT                                                  DOM03220
      FOLD = FNEW                                                       DOM03230
      ROLD = RNEW                                                       DOM03240
100   CONTINUE                                                          DOM03250
      VTOT = RHO2*RHO2 - RHO1*RHO1                                      DOM03260
      EPS = SUM                                                         DOM03270
      EPS = 2.0*EPS/VTOT                                                DOM03280
      RETURN                                                            DOM03290
      END                                                               DOM03300
C                                                                       DOM03310
      FONCTION EFUNC(R, DTDP, EBAR)                                     DOM03320
      PI = 2.0*ARSIN(1.0)                                               DOM03330
      A1 = 0.3463                                                       DOM03340
      A2 = 0.4273                                                       DOM03350
      A3 = 2.4509                                                       DOM03360
      A4 = 2.2011                                                       DOM03370
      Y = 0.5*DTDP*(1.0-R)                                              DOM03380
      IF( Y .LT. 0.25) GOTO 100                                         DOM03390
      YY = COS( (A3*Y-A4)*PI )                                          DOM03400
      YY = A1*YY/EXP(A2*Y)                                              DOM03410
      EFUNC = (1.0-EBAR)*YY + EBAR                                      DOM03420
      GOTO 1000                                                         DOM03430
100   CONTINUE                                                          DOM03440
C  THIS SECTION FOR 'WALL' REGION                                       DOM03450
      YY = 7.0*Y*Y/9.0                                                  DOM03460
      YY = 4.5*(Y-YY)                                                   DOM03470
      YY = (1.0-EBAR)*YY                                                DOM03480
      EFUNC = 1.0-YY                                                    DOM03490
1000  RETURN                                                            DOM03500
      END                                                               DOM03510
C                                                                       DOM03520
      SOBROUTINE FINDF(R,DIR,F)                                         DOM03530
C  DIRECT SEARCH FOR ROOT OF POLYNOMIAL.                                DOM03540
C  WILL LIMIT TO F BETWEEN 1 AND 5                                      DOM03550
C  WILL SEARCH IN INCREMENTS OF 0.01                                    DOM03560
      DELF = 0.005                                                      DOM03570
      F = 1.0-DELF                                                      DOM03580
10    F = F + DELF                                                      DOM03590
      IF(F .LE. 5.0)GOTO 20                                             DOM03600
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C  CAN'T FIND ROOT OF EQ'N; ABORT PROGRAM                                DUM03210
       WRITE(6,15)N,D1R                                                 DUM03220
15     FORMAT(' ***** PGM ABORTED IN SUBROUTINE FINDF.',/,              DUM03230
      1 'NO ROOT TO POLINOMIAL FOR N=',I3,' D1/R=',E11.4)               DUM03240
       STOP                                                             DUM03250
20     SUM = 1.0                                                        DUM03260
       TERM = 1.0                                                       DUM03270
       DO 30 I=2,N                                                      DUM03280
       TERM = TERM * F                                                  DUM03290
       SUM = SUM + TERM                                                 DUM03300
30     CONTINUE                                                         DUM03310
       TEST = 1.0/D1R                                                   DUM03320
       IF(SUM .GE. TEST)GOTO 100                                        DUM03330
       GOTO 10                                                          DUM03340
100    RETURN                                                           DUM03350
       END                                                              DUM03360
C                                                                       DUM03370
       SUBROUTINE MIX1(NA,NB,Q, W)                                      DUM03380
C  THIS SUBROUTINE DETERMINES WEIGHT FACTORS FOR                        DUM03390
C  MIXING AT ANNULUS INLETS                                             DUM03400
       DIMENSION Q(100),W(100)                                          DUM03410
       N = NA+NB                                                        DUM03420
       IF(NA .LE. NB) GOTO 200                                          DUM03430
C  THIS SECTION FOR NA GT NB                                            DUM03440
C  NEED WEIGHTS FOR ODD NUMBERED SEGMENTS                               DUM03450
       W(N) = 0.0                                                       DUM03460
       W(1) = 1.0                                                       DUM03470
       N2 = N-2                                                         DUM03480
       DO 10 I=3,N2,2                                                   DUM03490
       I1 = N2 - I + 3                                                  DUM03500
       W(I1) = ( Q(I1+1) - (1.0-W(I1+2))*Q(I1+2) )/Q(I1)                DUM03510
10     CONTINUE                                                         DUM03520
       GOTO 1000                                                        DUM03530
200    CONTINUE                                                         DUM03540
C  THIS SECTION FOR NA = NB                                             DUM03550
C  NEED WEIGHTS FOR EVEN NUMBERED SEGMENTS                              DUM03560
       W(N) = 0.0                                                       DUM03570
       N2 = N-2                                                         DUM03580
       DO 300 I=2,N2,2                                                  DUM03590
       I1 = 2-I+N2                                                      DUM03600
       W(I1) = ( Q(I1+1) - (1.0-W(I1+2))*Q(I1+2) )/Q(I1)                DUM03610
300    CONTINUE                                                         DUM03620
1000   CONTINUE                                                         DUM03630
       RETURN                                                           DUM03640
       END                                                              DUM03650
       SUBROUTINE MIX2(ITBANS,NA,NB,Q,W,C)                              DUM03660
       DIMENSION W(100),Q(100),C(100)                                   DUM03670
C  THIS SUBROUTINE DETERMINES ANNULUS INLET CONCENTRATIONS              DUM03680
C  ITBANS=0==>A TO B TRANSITION                                         DUM03690
C        =1==>B TO A TRANSITION                                         DUM03700
       N = NA+NB                                                        DUM03710
       IF(NA .LE. NB)GOTO 500                                           DUM03720
C  THIS SECTION FOR NA GT NB                                            DUM03730
       IF(ITBANS .NE. 0)GOTO 200                                        DUM03740
C  A TO B TBANS                                                         DUM03750
C  B'S ARE EVEN NUMBERED SUBSCRIPTS                                     DUM03760
       N1 = N-1                                                         DUM03770
       DO 100 I=2,N1,2                                                  DUM03780
       C(I) = (1.0-W(I+1))*Q(I+1)*C(I+1)                                DUM03790
       C(I) = C(I) + W(I-1)*Q(I-1)*C(I-1)                               DUM03800
       C(I) = C(I) / Q(I)                                               DUM03810
100    CONTINUE                                                         DUM03820
       RETURN                                                           DUM03830
200    CONTINUE                                                         DUM03840
C  B TO A TBANS                                                         DUM03850
C  A'S ARE ODD NUMBERED SUBSCRIPTS                                      DUM03860
       C(1) = C(2)                                                      DUM03870
       C(N) = C(N-1)                                                    DUM03880
       N2 = N-2                                                         DUM03890
       DO 300 I=3,N2,2                                                  DUM03900
       C(I) = (1.0-W(I))*C(I-1) + W(I)*C(I+1)                           DUM03910
300    CONTINUE                                                         DUM03920
       RETURN                                                           DUM03930
500    CONTINUE                                                         DUM03940
C  THIS SECTION FOR NA=NB                                               DUM03950
       IF(ITBANS .NE. 0)GOTO 700                                        DUM03960
C  A TO B TBANS                                                         DUM03970
C  B'S ODD NUMBERED SUBSCRIPTS                                          DUM03980
       C(1) = C(2)                                                      DUM03990
       N1 = N-1                                                         DUM04000
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      DO 600 I=3,N1,2                                                   COMM04010
      C(I) = (1.0-W(I+1))*Q(I+1)*C(I+1)                                 COMM04020
      C(I) = C(I) + W(I-1)*Q(I-1)*C(I-1)                                COMM04030
      C(I) = C(I) / Q(I)                                                COMM04040
600   CONTINUE                                                          COMM04050
      RETURN                                                            COMM04060
700   CONTINUE                                                          COMM04070
C  Q TO A TRANSITION                                                    COMM04080
C  A'S EVEN NUMBERED SUBSCRIPTS                                         COMM04090
      C(N) = C(N-1)                                                     COMM04100
      N2 = N-2                                                          COMM04110
      DO 800 I=2,N2,2                                                   COMM04120
      C(I) = W(I)*C(I+1) + (1.0-W(I))*C(I-1)                            COMM04130
800   CONTINUE                                                          COMM04140
      RETURN                                                            COMM04150
      END                                                               COMM04160
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      SOBROUTINE ANN(NA,NB,Q,B,A,B1,B2,BA,BB)                          DUB04170
      DIMENSION BA(100),BB(100)                                        DUB04180
      DIMENSION Q(100),R(100),RR(100),A(100)                           DUB04190
C  CALC  HYDRAULIC RADII, ABD AREAS                                     DUB04200
      N = NA + NB                                                      DUB04210
C  A HALF-CELL                                                         DUB04220
      DO 10 I=2,N,2                                                    DUB04230
      RR(I) = R(I) - RA(I-1)                                           DUB04240
      A(I) = R(I)*R(I) - RA(I-1)*RA(I-1)                               DUB04250
10    CONTINUE                                                         DUB04260
C  B HALF-CELL                                                         DUB04270
      RR(1) = RB(1)                                                    DUB04280
      A(1) = RR(1)*RB(1)                                               DUB04290
      NAI = N-1                                                        DUB04300
      DO 20 I=3,NAI,2                                                  DUB04310
      RR(I) = RR(I) - R(I-1)                                           DUB04320
      A(I) = RR(I)*RR(I) - R(I-1)*R(I-1)                               DUB04330
20    CONTINUE                                                         DUB04340
C  NOW, DETERMINE FLOWS AND POROSITIES OF A AND B SEGS                 DUB04350
C  DEPENDS ON NA AND NB                                                DUB04360
C ******                                                             DUB04370
C  ASSUME NA = NB                                                      DUB04380
C                                                                      DUB04390
C  THIS SECTION FOR NA=NB                                              DUB04400
C  FLOW DISTRIBUTION AND POROSITY                                      DUB04410
C  A-SEGMENT                                                           DUB04420
      SOA = 0.0                                                        DUB04430
      A1 = 0.0                                                         DUB04440
      DO 510 I=2,N,2                                                   DUB04450
      A1 = A1 + A(I)                                                   DUB04460
510   SOA = SOA + A(I)*RR(I)*RB(I)                                     DUB04470
      DO 520 I=2,N,2                                                   DUB04480
      Q(I) = A(I)*RR(I)*RB(I)/SOA                                      DUB04490
520   CONTINUE                                                         DUB04500
C  B-SEG                                                               DUB04510
C  USE FACTOR TO ACCOUNT FOR WEIRD RESISTANCES AT WALL AND C.L.        DUB04520
      A2 = 0.0                                                         DUB04530
      SOB = 0.0                                                        DUB04540
      N1 = N-1                                                         DUB04550
      DO 530 I=1,N1,2                                                  DUB04560
      A2 = A2+A(I)                                                     DUB04570
530   CONTINUE                                                         DUB04580
C  ----WALL RESISTANCES---                                             DUB04590
      FACTOR = 1.0                                                     DUB04600
      XX = A(B-1)*RR(B-1)*RR(B-1)                                      DUB04610
      YY = A(B-3)*RR(B-3)*RR(B-3)                                      DUB04620
      STUFF = Q(B-2) * XX/(XX + FACTOR*YY)                             DUB04630
      Q(B-1) = Q(B) + STUFF                                            DUB04640
      XX = A(B-3)*RR(B-3)*RR(B-3)                                      DUB04650
      YY = A(B-5)*RR(B-5)*RR(B-5)                                      DUB04660
      Q(B-3) = Q(B-2) - STUFF + Q(B-4)*XX/(XX+YY)                      DUB04670
C  -----CENTERLINE RESISTANCES---                                      DUB04680
      FACTOR = 1.0                                                     DUB04690
      XX = A(1)*RR(1)*RR(1)                                            DUB04700
      YY = A(3)*RR(3)*RR(3)                                            DUB04710
      Q(1) = Q(2)*XX*FACTOR/(XX*FACTOR + YY)                           DUB04720
      XX = A(3)*RR(3)*RR(3)                                            DUB04730
      YY = A(5)*RR(5)*RR(5)                                            DUB04740
      Q(3) = Q(2) - Q(1) + Q(4)*XX/(XX+YY)                             DUB04750
      NAX = N-5                                                        DUB04760
C  CAN'T HANDLE ANYTHING LESS THAN 8 RADIAL DIVS...                    DUB04770
      IF( N .LE. 6)GOTO 550                                            DUB04780
      DO 540 I=5,NAX,2                                                 DUB04790
      XX = A(I)*RR(I)*RR(I)                                            DUB04800
                                                                       DUB04810
      YY = A(I-2)*RR(I-2)*RR(I-2)                                      DUB04820
      ZZ = A(I+2)*RR(I+2)*RR(I+2)                                      DUB04830
      Q(I) = Q(I-1)*ZZ/(XX+YY) + Q(I+1)*XX/(XX+ZZ)                     DUB04840
540   CONTINUE                                                         DUB04850
      GOTO 1000                                                        DUB04860
550   CONTINUE                                                         DUB04870
      WRITE(6,560)                                                     DUB04880
560   FORMAT('------PGM ABORT IN -ANN-.  N .LT. 8.....')              DUB04890
1000  RETURN                                                           DUB04900
      END
```

Transient Mass Dispersion

General program flow builds a time step loop around the steady-state calculations. Concentration becomes a triple-subscripted array as explained in the listing. Additional subroutines are:

1. STEP--shifts delay time arrays;
2. DELTA--determines number of delay elements (time steps) NSUB (I) corresponding to each radial plug.

Variables (TDEAD(I) correspond to delay times. Additional information is provided by the comments contained within the listing. All time variables are scaled by bed hold-up time (ignore any spurious comment statements in the listing to the contrary).

```
C  PROGRAM NAME 'PLSV3 FORTRAN'                                          FLS00010
C                                                                        FLS00020
C  ---------------------------------------------------                   FLS00030
C  THIS SUB FOR DATA OF CAIRNS AND FRAUSNITZ                             FLS00040
C  ---------------------------------------------------                   FLS00050
C                                                                        FLS00060
C  LAST UPDATE/USE ON 30 APR 85                                          FLS00070
C                                                                        FLS00080
C  TRANSIENT AAP MODEL                                                   FLS00090
C  SUBSCRIPTS ON C(I,J,K)--                                              FLS00100
C        I=RADIAL POSITION                                               FLS00110
C        J=AXIAL POS (A/B CELL NO.)                                      FLS00120
C        K=TIME STEPS (FOR DEAD TIME PURPOSES)                           FLS00130
      COMMON /ONE/ RA(21),RB(21),R(20)                                   FLS00140
      COMMON /TWO/ Q(20), A(20), W(20)                                   FLS00150
      COMMON /FIVE/ C(20,118,50), CIN(20,118)                            FLS00160
      COMMON /FOUR/ TDEAD(20),NSUB(20)                                   FLS00170
      DIMENSION ODMNT(20),TBL(20),EPS(20)                                FLS00180
C                                                                        FLS00190
C  IOPT       =0--PRINT ONLY AVG CONC AT EACH TPRINT                     FLS00200
C             =ANYTHING ELSE, PRINT EVERYTHING AT EACH TPRINT            FLS00210
C                                                                        FLS00220
      DATA IOPT /0/                                                      FLS00230
C                                                                        FLS00240
C                                                                        FLS00250
C                                                                        FLS00260
C  ---------------------------------------------------------------------FLS00270
C  THIS SECTION SIZES ABNORL, CALCS FLOWS, VELOCITIES, ETC.              FLS00280
C                                                                        FLS00290
C                                                                        FLS00300
C  ---------------------------------------------------------------------FLS00310
C                                                                        FLS00320
C  CALC AREAS BASED ON OIOP AND EA                                       FLS00330
      DIDP = 15.9                                                        FLS00340
      DO 10 I=1,20                                                       FLS00350
10    W(I) = 20.0                                                        FLS00360
C  NOW, THEY ASSIGNING NO. CELLS BASED ON CORRELATION...                 FLS00370
      Z = DIDP/0.816 + 0.5                                               FLS00380
      N = Z                                                              FLS00390
      Z = N                                                              FLS00400
      Z = 0.5*Z                                                          FLS00410
      NB = Z                                                             FLS00420
      NA = N-NB                                                          FLS00430
C  RESTRICT TO EVEN NO. SEGMENTS                                         FLS00440
      IF(NA .GT. NB)NB = NA                                              FLS00450
      N = NA+NB                                                          FLS00460
      WRITE(6,3020)DIDP,N,NA,NB                                          FLS00470
C  SIZE RADII                                                            FLS00480
C  SET UP TO DO INCREASING EA'S...                                       FLS00490
C  SIZE EVENLY SPACED RADII                                              FLS00500
      ZN = N/2                                                           FLS00510
      DELR = 1.0/ZN                                                      FLS00520
      R(2) = DELR                                                        FLS00530
      DO 80 I=4,N,2                                                      FLS00540
      R(I) = R(I-2) + DELR                                               FLS00550
80    CONTINUE                                                           FLS00560
C  DETERMINE EPS FOR EACH SEGMENT...                                     FLS00570
      EBAR = 0.360                                                       FLS00580
C  VOID FRACTION OF FIRST SEGMENT                                        FLS00590
      CALL VOID(100,DIDP,0.0,R(2),EBAR,E1)                               FLS00600
      I=2                                                                FLS00610
      WRITE(6,3010)I,E1                                                  FLS00620
C                                                                        FLS00630
C **********  TEST--LOWER VELOCITY BY MULT TIMES POROSITY **********     FLS00640
      EPS(2) = E1                                                        FLS00650
      EPS(1) = E1                                                        FLS00660
100   RA(1) = (1.0-E1)*R(2)*R(2)                                         FLS00670
      RA(1) = SQRT( RA(1) )                                              FLS00680
      RB(1) = E1*R(2)*R(2)                                               FLS00690
      RB(1) = SQRT( RB(1) )                                              FLS00700
      NAI = N-1                                                          FLS00710
      DO 120 I=3,NAI,2                                                   FLS00720
C  VOID FRACTIONS OF RADIAL CELLS BASED ON CORRELATION                   FLS00730
      RHO2 = R(I+1)                                                      FLS00740
      RHO1 = R(I-1)                                                      FLS00750
      CALL VOID(100,DIDP,RHO1,RHO2,EBAR,EHAT)                            FLS00760
      IW = I+1                                                           FLS00770
      WRITE(6,3010)IW,EHAT                                               FLS00780
      EPS(IW) = EHAT                                                     FLS00790
      EPS(I) = EHAT                                                      FLS00800
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      XI = R(I+1)*B(I+1) - R(I-1)*B(I-1)                                FLS00810
      BA(I) = (1.0-EPAT)*XI                                             FLS00820
      BA(I) = R(I-1)*B(I-1) + BA(I)                                     FLS00830
      BA(I) = SQRT( BA(I) )                                             FLS00840
      BB(I) = ZMAT * XI                                                 FLS00850
      BB(I) = R(I-1)*B(I-1) + BB(I)                                     FLS00860
      BB(I) = SQRT( BB(I) )                                             FLS00870
  120 CONTINUE                                                          FLS00880
      NAX = N-1                                                         FLS00890
      WRITE(6,3150)                                                     FLS00900
      WRITE(6,3160) (BA(I),R(I+1),I=1,NAX,2)                            FLS00910
      WRITE(6,3160) (BB(I),R(I+1),I=1,NAX,2)                            FLS00920
      CALL ANN(NA,BB,E1,E2)                                             FLS00930
      N = NA+NB                                                         FLS00940
CCC   DO 200 I=1,N                                                      FLS00950
C200  VEL(I) =  Q(I)/A(I)                                               FLS00960
C*****************************************************************    FLS00970
C  TEST CALCULATING VELOCITY BY SIMPLE RATIO OF EPS/EDAR...           *FLS00980
C*****************************************************************    FLS00990
      DO 210 I=1,N                                                      FLS01000
CCC   VEL(I) = EPS(I)/E1                                                FLS01010
CCC   VEL(I) = VEL(I)*VEL(I)                                            FLS01020
C  *-*-*-*-* BACK TO OLD WAY *-*-*-*                                    FLS01030
      VEL(I) = E1*Q(I)/A(I)                                             FLS01040
  210 CONTINUE                                                          FLS01050
C  WRITE RESULTS                                                        FLS01060
      WRITE(6,3050)                                                     FLS01070
      IF( NA .GT. NB)GOTO 390                                           FLS01080
      DO 300 I=2,N,2                                                    FLS01090
      J=I-1                                                             FLS01100
      WRITE(6,3060) I,A(I),Q(I),VEL(I),J,A(J),Q(J),VEL(J)               FLS01110
  300 CONTINUE                                                          FLS01120
      WRITE(6,3070) E1,E2                                               FLS01130
      GOTO 410                                                          FLS01140
  390 CONTINUE                                                          FLS01150
      NAX = N-1                                                         FLS01160
      DO 400 I=1,NAX,2                                                  FLS01170
      J = I+1                                                           FLS01180
      WRITE(6,3060) I,A(I),Q(I),VEL(I),J,A(J),Q(J),VEL(J)               FLS01190
  400 CONTINUE                                                          FLS01200
      WRITE(6,3060) N,A(N),Q(N),VEL(N)                                  FLS01210
      WRITE(6,3070) E1,E2                                               FLS01220
  410 CONTINUE                                                          FLS01230
      WRITE(6,3150)                                                     FLS01240
      WRITE(6,3160) (R(I),I=1,N)                                        FLS01250
      CALL MIX1(NA,NB)                                                  FLS01260
      WRITE(6,3170)                                                     FLS01270
      WRITE(6,3160) (W(I),I=1,N)                                        FLS01280
C                                                                       FLS01290
C ----------------------------------------------------------------------FLS01300
C                                                                       FLS01310
C  THIS SECTION TAKES CARE OF TIME STEPS, ETC.                          FLS01320
C                                                                       FLS01330
C ----------------------------------------------------------------------FLS01340
C                                                                       FLS01350
      DTINE = 5.0E-4                                                    FLS01360
      TMAX = 1.13                                                       FLS01370
C  SET OF FOLSE WIDTH                                                   FLS01380
      WIDTH = TMAX+DTINE                                                FLS01390
C  ------NOTE THAT ABOVE ENSURES STEP INPUT                            FLS01400
      TPRINT = 0.005                                                    FLS01410
      NPRINT = TPRINT / DTINE                                           FLS01420
      WRITE(6,1015) DTINE                                               FLS01430
1015  FORMAT(22,'DTINE =',E11.4)                                        FLS01440
      NZMAX = 117                                                       FLS01450
C                                                                       FLS01460
C  CALC GRAD TIMES BASED ON VELOCITIES.  NOTE--TREY'RE                  FLS01470
C     IN INTERVALS OF BOLD-UP TIMES.                                    FLS01480
C                                                                       FLS01490
      KIZ = NZMAX                                                       FLS01500
      DO 1020 II=1,N                                                    FLS01510
CCC   TGRAD(II) = 1.0 / (2.0 * KIZ * E1  * VEL(II) )                    FLS01520
C  USE REAL(DIMENSIONAL) TIME...                                        FLS01530
C  TIME IN SEC, DI AND DP IN INCHES                                     FLS01540
C  QTOT IN CU.IN/SEC                                                    FLS01550
CCC   QTCT = 11.55 * 2.0/3.0                                            FLS01560
CCC   DP = 0.75                                                         FLS01570
CCC   DT = DTDP*DP                                                      FLS01580
CCC   CL = 0.816 * DP                                                   FLS01590
CCC   AIS = 3.14 * DT * DT / 4.0                                        FLS01600
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CCC     TDEAD(II) = CL * AIS / ( YEL(II)*QTOT )                          PLS01610
        XIZ = NZMAX                                                      PLS01620
        TDEAD(II) = 1.0/( YEL(II)*2.0*XIZ )                              PLS01630
 1020   CONTINUE                                                         PLS01640
        CALL DELTA(DTIME, N, NA, NB, JMAX, MCHG)                         PLS01650
        WRITE(6,1016) (I,TDEAD(I),NSUB(I),I=1,N)                         PLS01660
 1016   FORMAT(15,2X,B11.4,I5)                                           PLS01670
        IFLAG = 0                                                        PLS01680
C  IFLAG =0==>INLET CONC'N = 1.0                                         PLS01690
C        .NE.0==>INLET CONC'N = 0.0                                      PLS01700
C                                                                        PLS01710
        CALL STEP(N,NA,NB,TIME,IFLAG)                                    PLS01720
        TIME = 0.0                                                       PLS01730
CCC     NSP = JMAX                                                       PLS01740
        KOUNT = 0                                                        PLS01750
        IPRINT = 0                                                       PLS01760
        JMAX = NZMAX                                                     PLS01770
 1050   CONTINUE                                                         PLS01780
C  FOR TESTING, WRITE BEG INLET CONC'NS                                  PLS01790
C  ASSUME CALL EVEN NO. RADIAL DIVISIONS                                 PLS01800
CCC     WRITE(6,3270)                                                    PLS01810
CCC     DO 1051 I=2,N,2                                                  PLS01820
CCC     ISUB = NSUB(I)                                                   PLS01830
CCC     WRITE(6,3160)CIN(I,1), C(I,1,ISUB)                               PLS01840
C 1051  CONTINUE                                                         PLS01850
C  SET UP FOLSE UP STEP                                                  PLS01860
        IF(TIME .GT. WIDTH)IFLAG = 10                                    PLS01870
        DO 1100 J=1,JMAX                                                 PLS01880
C  B INLETS==>A OUTLETS, ETC.                                            PLS01890
C  OUTLETS==>SUBSCRIPT=1;  INLETS==>SUBSCRIPT=NSUB                       PLS01900
C  TRANSFER TO DUMMY ARRAY TO USE SUBROUTINE                             PLS01910
C  A TO B TRANSITION...                                                  PLS01920
        DO 1060 I=1,N,2                                                  PLS01930
C  THIS PART NA=NB                                                       PLS01940
        IA = I+1                                                         PLS01950
        IB = I                                                           PLS01960
 1060   OUBBI(IA) = C(IA,J,1)                                            PLS01970
        CALL MIX2(0,NA,NB,DUMMY)                                         PLS01980
C  TRANSFER TO CIN ARRAY                                                 PLS01990
        DO 1070 I=1,N,2                                                  PLS02000
C  THIS PART NA=NB                                                       PLS02010
        IA = I+1                                                         PLS02020
        IB = I                                                           PLS02030
 1070   CIN(IB,J) = DUMMY(IB)                                            PLS02040
C  B TO A TRANSITION                                                     PLS02050
        DO 1080 I=1,N,2                                                  PLS02060
C  THIS SET NA=NB                                                        PLS02070
        IA = I+1                                                         PLS02080
        IB = I                                                           PLS02090
 1080   DUMMY(IB) = C(IB,J,1)                                            PLS02100
        CALL MIX2(1,NA,NB,DUMMY)                                         PLS02110
C  BACK TO CIN'S                                                         PLS02120
        DO 1090 I=1,N,2                                                  PLS02130
C  NA = NB                                                               PLS02140
        IA = I+1                                                         PLS02150
        IB = I                                                           PLS02160
 1090   CIN(IA,J+1) = OUBBI(IA)                                          PLS02170
 1100   CONTINUE                                                         PLS02180
C  SHIFT ARRAYS FOR NEXT TIME                                            PLS02190
C  DON'T FORGET TO CHECK IF WE NEED FOLSE INPUT                          PLS02200
        IF(IFLAG .EQ. 0)GOTO 1110                                        PLS02210
        CALL STEP(N,NA,NB,TIME,IFLAG)                                    PLS02220
 1110   CONTINUE                                                         PLS02230
        DO 1200 J=1,JMAX                                                 PLS02240
        DO 1200 I=1,N                                                    PLS02250
        KMAX = NSUB(I) - 1                                               PLS02260
        DO 1150 K=1,KMAX                                                 PLS02270
        K1 = K+1                                                         PLS02280
        C(I,J,K) = C(I,J,K1)                                             PLS02290
 1150   CONTINUE                                                         PLS02300
C  NOW, INLETS GO INTO LAST POSITION                                     PLS02310
        K1 = NSUB(I)                                                     PLS02320
        C(I,J,K1) = CIN(I,J)                                             PLS02330
 1200   CONTINUE                                                         PLS02340
C  ONLY WRITE RESULTS AT DESIRED INTERVALS                               PLS02350
        IPRINT = IPRINT + 1                                              PLS02360
        IF(IPRINT .LT. NPRINT)GOTO 1350                                  PLS02370
        IPRINT = 0                                                       PLS02380
C  CHECK IF WE WRITE EVERYTHING OR ONLY AVG.                             PLS02390
        IF(IOPT .EQ. 0)GOTO 1305                                         PLS02400
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1230  CONTINUE                                                          FLS02410
      WRITE(6,2060)TIME                                                 FLS02420
C  NOW PRINT RESULS (OUTLET FROM EACH CELL)                             FLS02430
      DO 1300 J=1,JMAX                                                  FLS02440
      DO 1250 I=2,N,2                                                   FLS02450
      IF(NA .LE. NB)GOTO 1240                                           FLS02460
C  NA>NB                                                               FLS02470
      IA = I-1                                                          FLS02480
      IB = I                                                            FLS02490
      GOTO 1245                                                         FLS02500
1240  CONTINUE                                                          FLS02510
C  NA=NB                                                               FLS02520
      IA = I                                                            FLS02530
      IB = I-1                                                          FLS02540
1245  WRITE(6,2050)IA,C(IA,J,1),IB,C(IB,J,1)                            FLS02550
1250  CONTINUE                                                          FLS02560
      IF(NA .GT. NB)WRITE(6,2050)N,C(N,J,1)                             FLS02570
1300  CONTINUE                                                          FLS02580
1305  CONTINUE                                                          FLS02590
C                                                                       FLS02600
C  CALC AVG CONC OVER CROSS-SECTION OF LAST CELL                        FLS02610
C       (N IS OUTLET)                                                   FLS02620
C                                                                       FLS02630
      XIZ = 0.0                                                         FLS02640
      IF(NA .LE. NB) GOTO 1315                                          FLS02650
C  THIS PART NA GT NB                                                  FLS02660
      DO 1310 I=2,N,2                                                   FLS02670
      TERM = C(I,JMAX,1) * Q(I)                                         FLS02680
      XIZ = XIZ + TERM                                                  FLS02690
1310  CONTINUE                                                          FLS02700
      GOTO 1330                                                         FLS02710
1315  CONTINUE                                                          FLS02720
C  THIS PART NA=NB                                                     FLS02730
      DO 1320 I=1,N,2                                                   FLS02740
      TERM = C(I,JMAX,1) * Q(I)                                         FLS02750
      XIZ = XIZ + TERM                                                  FLS02760
1320  CONTINUE                                                          FLS02770
1330  CONTINUE                                                          FLS02780
C  NOW WRITE AVG CONCENTRATION                                         FLS02790
      WRITE(6,3260)TIME,XIZ                                             FLS02800
1350  CONTINUE                                                          FLS02810
1600  CONTINUE                                                          FLS02820
C  CHECK TIME                                                          FLS02830
      IF(TIME .GE. TMAX)GOTO 10000                                      FLS02840
      TIME = TIME + DTIME                                               FLS02850
      GOTC 1050                                                         FLS02860
C  FORMATS...                                                          FLS02870
2050  FORMAT(2 (I4,2X,E11.4,4X) )                                       FLS02880
2060  FORMAT(/,' TIME = ',E11.4)                                        FLS02890
C2070  FORMAT(' GROUP NO. ',I4)                                         FLS02900
2080  FORMAT(' -----FLIP/FLOPPED CELLS-----')                           FLS02910
2090  FORMAT(' -----AT TIME = ',E11.4,'  (AND LESS) ',/,                FLS02920
     1 '          LAST CELL NO. IS ',I5)                               FLS02930
3010  FORMAT(' I =',I4,'  EPS = ',E11.4)                                FLS02940
3020  FORMAT(' DTOP = ',E11.4,'  N =',I3,' NA =',I3,' NB =',I3)         FLS02950
3050  FORMAT(20X,'A',83X,'B',/,2X,40('-'),2X,40('-'),/,                 FLS02960
     1 2(2X,'I',7X,'A',11X,'F',9X,'FL  ',5X),/,                         FLS02970
     2 1X,2('---',2X,3('----------',2X)))                               FLS02980
3060  FORMAT(1X,2(I3,2X,3(E10.4,2X)))                                   FLS02990
3070  FORMAT(' E1 = ',E11.4,'  E2 = ',E11.4)                            FLS03000
3150  FORMAT(' BADIA...')                                               FLS03010
3160  FORMAT(5(2X,E11.4))                                               FLS03020
3170  FORMAT(' MIXING WEIGHT FACTORS. . .')                             FLS03030
3230  FORMAT(9X,'A',30X,'B',/,2(2X,29('-')),/,                          FLS03040
     1 3X,2(1X,'I',8X,'C',7X,3X,'C/CAVG',8X),/,                         FLS03050
     2 2X,2('---',2X,'----------',2X,'----------',2X))                  FLS03060
C33456789.123456789.123456789.123456789.123456789.                     FLS03070
3240  FORMAT(' CELL NO ',I5)                                            FLS03080
3250  FORMAT(2X,2(I3,2X,E11.4,2X,E11.4,2X))                             FLS03090
3260  FORMAT(1X,'TIME = ',E11.4,3X,'AVG CONC IS ',E11.4)                FLS03100
3270  FORMAT(' CIN(I,1)...C(I,1,850) ')                                 FLS03110
10000 CONTINUE                                                          FLS03120
      STCP                                                              FLS03130
      END                                                               FLS03140
      SOBROUTINE ANB(NA,NB,E1,E2)                                       FLS03150
      COMMCN /OBE/ BA(21),BB(21),B(20)                                  FLS03160
      COMMCN /TWO/ Q(20),A(20),W(20)                                    FLS03170
      DIMENSION BB(20)                                                  FLS03180
C  CALC  HYDRAULIC BADII, AND AREAS                                     FLS03190
      B = BA + BB                                                       FLS03200
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C   A HALF-CELL                                                          FLS03210
      DO 10 I=2,N,2                                                      FLS03220
      BB(I) = B(I) - BA(I-1)                                             FLS03230
      A(I) = B(I)*B(I) - BA(I-1)*BA(I-1)                                 FLS03240
10    CONTINUE                                                           FLS03250
C   B HALF-CELL                                                          FLS03260
      BB(1) = BB(1)                                                      FLS03270
      A(1) = BB(1)*BB(1)                                                 FLS03280
      MAX = N-1                                                          FLS03290
      DO 20 I=3,MAX,2                                                    FLS03300
      BB(I) = BB(I) - B(I-1)                                             FLS03310
      A(I) = BB(I)*BB(I) - B(I-1)*B(I-1)                                 FLS03320
20    CONTINUE                                                           FLS03330
C   NOW, DETERMINE FLOWS AND POROSITIES OF A AND B SEGS                  FLS03340
C   DEPENDS ON NA AND NB                                                 FLS03350
      IF(NA .LE. NB) GOTO 500                                            FLS03360
C   THIS SECTON FOR NA GT NB                                             FLS03370
C   FLOW DISTRIBUTION AND POROSITY                                       FLS03380
      S1 = 0.0                                                           FLS03390
      SUM = 0.0                                                          FLS03400
      DO 100 I=1,N,2                                                     FLS03410
      S1 = S1 + A(I)                                                     FLS03420
100   SUM = SUM + A(I)*SQRT(BB(I))                                       FLS03430
      DO 110 I=1,N,2                                                     FLS03440
      Q(I) = A(I)*SQRT(BB(I))/SUM                                        FLS03450
110   CONTINUE                                                           FLS03460
C   B SEGMENT                                                            FLS03470
      S2 = 0.0                                                           FLS03480
      SUM = 0.0                                                          FLS03490
      N1 = N-1                                                           FLS03500
      DO 120 I=2,N1,2                                                    FLS03510
      S2 = S2+A(I)                                                       FLS03520
120   CONTINUE                                                           FLS03530
      XX = A(N-1)*SQRT( BB(N-1) )                                        FLS03540
      YY = A(N-3)*SQRT( BB(N-3) )                                        FLS03550
      Q(N-1) = Q(N) * Q(N-2) *XX/(XX+YY)                                 FLS03560
      XX = A(2)*SQRT(BB(2))                                              FLS03570
      YY = A(4)*SQRT(BB(4))                                              FLS03580
      Q(2) = Q(1) + Q(3)*XX/(XX+YY)                                      FLS03590
      MAX = N-3                                                          FLS03600
C   DON'T NEED FOLLOWING IF N .LE. 5                                     FLS03610
      IF(N .LE. 5)GOTO 1000                                              FLS03620
      DO 130 I=4,MAX,2                                                   FLS03630
      XX = A(I)*SQRT(BB(I))                                              FLS03640
      YY = A(I-2)*SQRT(BB(I-2))                                          FLS03650
      ZZ = A(I+2)*SQRT(BB(I+2))                                          FLS03660
      Q(I) = Q(I-1)*XX/(XX+YY) + Q(I+1)*XX/(XX+ZZ)                       FLS03670
130   CONTINUE                                                           FLS03680
      GOTO 1000                                                          FLS03690
500   CONTINUE                                                           FLS03700
C   THIS SECTION FOR NA=NB                                               FLS03710
C   FLOW DISTRIBUTION AND POROSITY                                       FLS03720
C   A-SEGMENT                                                            FLS03730
      SUM = 0.0                                                          FLS03740
      S1 = 0.0                                                           FLS03750
      DO 510 I=2,N,2                                                     FLS03760
      S1 = S1 + A(I)                                                     FLS03770
510   SUM = SUM + A(I)*SQRT(BB(I))                                       FLS03780
      DO 520 I=2,N,2                                                     FLS03790
      Q(I) = A(I)*SQRT(BB(I))/SUM                                        FLS03800
520   CONTINUE                                                           FLS03810
C   B-SEG                                                                FLS03820
      S2 = 0.0                                                           FLS03830
      SUM = 0.0                                                          FLS03840
      N1 = N-1                                                           FLS03850
      DO 530 I=1,N1,2                                                    FLS03860
      S2 = S2+A(I)                                                       FLS03870
530   CONTINUE                                                           FLS03880
      XX = A(N-1)*SQRT(BB(N-1))                                          FLS03890
      YY = A(N-3)*SQRT(BB(N-3))                                          FLS03900
      Q(N-1) = Q(N) * Q(N-2) *XX/(XX+YY)                                 FLS03910
      XX = A(1)*SQRT(BB(1))                                              FLS03920
      YY = A(3)*SQRT(BB(3))                                              FLS03930
      Q(1) = Q(2)*XX/(XX+YY)                                             FLS03940
      MAX = N-3                                                          FLS03950
C   DON'T NEED FOLLOWINGIF N .LE. 4                                      FLS03960
      IF( N .LE. 4)GOTO 1000                                             FLS03970
      DO 540 I=3,MAX,2                                                   FLS03980
      XX = A(I)*SQRT(BB(I))                                              FLS03990
      YY = A(I-2)*SQRT(BB(I-2))                                          FLS04000
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      ZZ = A(I+2)*SQRT(RH(I+2))                                          FLS04010
      Q(I) = Q(I-1)*ZZ/(ZZ+YI) + Q(I+1)*ZZ/(ZZ+ZZ)                       FLS04020
  540 CONTINUE                                                           FLS04030
 1000 RETURN                                                             FLS04040
      END                                                                FLS04050
C                                                                        FLS04060
      SUBROUTINE XIZ2(ITRANS,NA,NB,C)                                    FLS04070
      COMMON /TWO/ Q(20),A(20),W(20)                                     FLS04080
      DIMENSION C(20)                                                    FLS04090
C  THIS SUBROUTINE OBTERMINES ANGULOS INLET CONCENTRATIONS              FLS04100
C  ITRANS=0==>A  TO B TRANSITION                                        FLS04110
C        =1==>B TO A TRANSITION                                         FLS04120
      N = NA+NB                                                          FLS04130
      IF(NA .LE. NB)GOTO 500                                             FLS04140
C  THIS SECTION FOR NA GT NB                                           FLS04150
      IF(ITRANS .NE. 0)GOTO 200                                          FLS04160
C  A TO B TRANS                                                        FLS04170
C  B'S ARE EVEN NUMBERED SUBSCRIPTS                                    FLS04180
      N1 = N-1                                                           FLS04190
      DO 100 I=2,N1,2                                                    FLS04200
      C(I) = (1.0-W(I+1))*Q(I+1)*C(I+1)                                  FLS04210
      C(I) = C(I) + W(I-1)*Q(I-1)*C(I-1)                                 FLS04220
      C(I) = C(I) / Q(I)                                                 FLS04230
  100 CONTINUE                                                           FLS04240
      RETURN                                                             FLS04250
  200 CONTINUE                                                           FLS04260
C  B TO A TRANS                                                        FLS04270
C  A'S ARE ODD NUMBERED SUBSCRIPTS                                     FLS04280
      C(1) = C(2)                                                        FLS04290
      C(N) = C(N-1)                                                      FLS04300
      N2 = N-2                                                           FLS04310
      DO 300 I=3,N2,2                                                    FLS04320
      C(I) = (1.0-W(I))*C(I-1) + W(I)*C(I+1)                             FLS04330
  300 CONTINUE                                                           FLS04340
      RETURN                                                             FLS04350
  500 CONTINUE                                                           FLS04360
C  THIS SECTION FOR NA=NB                                              FLS04370
      IF(ITRANS .NE. 0)GOTO 700                                          FLS04380
C  A TO B TRANS                                                        FLS04390
C  B'S ODD NUMBERED SUBSCRIPTS                                         FLS04400
      C(1) = C(2)                                                        FLS04410
      N1 = N-1                                                           FLS04420
      DO 600 I=3,N1,2                                                    FLS04430
      C(I) = (1.0-W(I+1))*Q(I+1)*C(I+1)                                  FLS04440
      C(I) = C(I) + W(I-1)*Q(I-1)*C(I-1)                                 FLS04450
      C(I) = C(I) / Q(I)                                                 FLS04460
  600 CONTINUE                                                           FLS04470
      RETURN                                                             FLS04480
  700 CONTINUE                                                           FLS04490
C  B TO A TRANSITION                                                   FLS04500
C  A'S EVEN NUMBERED SUBSCRIPTS                                        FLS04510
      C(N) = C(N-1)                                                      FLS04520
      N2 = N-2                                                           FLS04530
      DO 800 I=2,N2,2                                                    FLS04540
      C(I) = W(I)*C(I+1) + (1.0-W(I))*C(I-1)                             FLS04550
  800 CONTINUE                                                           FLS04560
      RETURN                                                             FLS04570
      END                                                                FLS04580
      SUBROUTINE STEP(W,NA,NB,TIME,IFLAG)                                FLS04590
      COMMON /FIVE/ C(20,118,50),CIN(20,118)                             FLS04600
      COMMON /FOUR/ IOEA0(20),NSUB(20)                                   FLS04610
      IF(TIME .GT. 0.0)GOTO 15                                           FLS04620
      DO 10 I=1,20                                                       FLS04630
      DO 10 J=1,118                                                      FLS04640
      DO 10 K=1,50                                                       FLS04650
      C(I,J,K) = 0.0                                                     FLS04660
   10 CONTINUE                                                           FLS04670
   15 CONTINUE                                                           FLS04680
C  NOW, SET UP STEP-CHANGE (OR POLSE) AT INLET                         FLS04690
C  IFLAG =0==>INLET CONC AT 1.0                                        FLS04700
C        = 1==>BACK TO 0.0                                             FLS04710
      VALUE = 1.0                                                        FLS04720
      IF(IFLAG .NE. 0)VALUE = 0.0                                        FLS04730
C                                                                        FLS04740
C  NOTE--ASSUME ONLY EVEN NO. RADIAL DIVISIONS                         FLS04750
C                                                                        FLS04760
C  THIS SECTION FOR NA = NB                                            FLS04770
  100 CONTINUE                                                           FLS04780
      DO 150 I=2,N,2                                                     FLS04790
      ISUB = NSUB(I)                                                     FLS04800
```

```
      C(I,1,ISUB) = VALUE                                              FLS04810
      CIB(I,1) = VALUE                                                 FLS04820
      IF(TIME .GT. 0.0)GOTO 145                                        FLS04830
      I1 = I-1                                                         FLS04840
      ISUB = NSUB(I1)                                                  FLS04850
      C(I1,1,ISUB) = 0.0                                               FLS04860
      CIB(I1,1) = 0.0                                                  FLS04870
145   CONTINUE                                                         FLS04880
150   CONTINUE                                                         FLS04890
      RETURN                                                           FLS04900
      END                                                              FLS04910
C                                                                      FLS04920
      SUBROUTINE GELTA(DTIME, N, NA, NB, JMAX, NCHG)                   FLS04930
      COMMON /FCUB/ TOEAQ(20),NSUB(20)                                 FLS04940
C  CALC TIME STEPS/DEAD TME                                            FLS04950
      DO 100 I=1,N                                                     FLS04960
      ZZZ = TOEAQ(I) / DTIME + 0.5                                     FLS04970
      NSUB(I) = ZZZ                                                    FLS04980
      IF(NSUB(I) .LT. 1) NSUB(I) = 1                                   FLS04990
100   CONTINUE                                                         FLS05000
C  NOW, CALC MAX AND MIN NSUB'S IN EACH HALF-CELL                      FLS05010
C  ...DEPENDS ON NA=NB OR NA>NB                                        FLS05020
      IF(NA .LE. NB) GOTO 500                                          FLS05030
C  THIS SECTON FOR NA>NB                                               FLS05040
      MAXA = 0                                                         FLS05050
      MAXB = 0                                                         FLS05060
      MINA = 1E6                                                       FLS05070
      MINB = 1E6                                                       FLS05080
      DO 200 I=1,N,2                                                   FLS05090
      IF(NSUB(I) .LT. MAXA)GOTO 150                                    FLS05100
      MAXA = NSUB(I)                                                   FLS05110
150   CONTINUE                                                         FLS05120
      IF(NSUB(I) .GT. MINA)GOTO 160                                    FLS05130
      MINA = NSUB(I)                                                   FLS05140
160   CONTINUE                                                         FLS05150
      I1 = I+1                                                         FLS05160
      IF(I1 .GT. N)GOTO 200                                            FLS05170
      IF(NSUB(I1) .LT. MAXB) GOTO 180                                  FLS05180
      MAXB = NSUB(I1)                                                  FLS05190
180   CONTINUE                                                         FLS05200
      IF(NSUB(I1) .GT. MINB) GOTO 200                                  FLS05210
      MINB = NSUB(I1)                                                  FLS05220
200   CONTINUE                                                         FLS05230
      GOTO 700                                                         FLS05240
C  THIS SECTION FOR NA=NB                                              FLS05250
500   CONTINUE                                                         FLS05260
      MAXA = 0                                                         FLS05270
      MAXB = 0                                                         FLS05280
      MINA = 1E6                                                       FLS05290
      MINB = 1E6                                                       FLS05300
      DO 600 I=2,N,2                                                   FLS05310
      IF(NSUB(I) .LT. MAXA)GOTO 550                                    FLS05320
      MAXA = NSUB(I)                                                   FLS05330
550   CONTINUE                                                         FLS05340
      IF(NSUB(I) .GT. MINA)GOTO 560                                    FLS05350
      MINA = NSUB(I)                                                   FLS05360
560   CONTINUE                                                         FLS05370
      I1 = I-1                                                         FLS05380
      IF(NSUB(I1) .LT. MAXB) GOTO 580                                  FLS05390
      MAXB = NSUB(I1)                                                  FLS05400
580   CONTINUE                                                         FLS05410
      IF(NSUB(I1) .GT. MINB) GOTO 600                                  FLS05420
      MINB = NSUB(I1)                                                  FLS05430
600   CONTINUE                                                         FLS05440
C                                                                      FLS05450
700   CONTINUE                                                         FLS05460
      WRITE(6,2000)MAXA,MAXB                                           FLS05470
      WRITE(6,2010) MINA, MINB                                         FLS05480
C  NOW, ADD UP MAX'S AND MIN'S TO CALC NO AXIAL CELLS (JMAX)           FLS05490
      NCHG = 0                                                         FLS05500
CCC   SMAX = MAXA + MAXB                                               FLS05510
CCC   SMIN = MINA + MINB                                               FLS05520
CCC   ZZZ = SMAX/SMIN                                                  FLS05530
CCC   JMAX = ZZZ                                                       FLS05540
CCC   JMAX = JMAX + 1                                                  FLS05550
CCC   NCHG = MAXA + MAXB                                               FLS05560
CCC   WRITE(6,2020)JMAX,NCHG                                           FLS05570
CCC   IF( JMAX .LE. (10) )GOTO 750                                     FLS05580
CCC   WRITE(6,2040)                                                    FLS05590
CCC   STOP                                                             FLS05600
```

```
      IFLAG = 0                                                         PLS03620
      DO 800 I=1,N                                                      PLS05630
      IF( NSOB(I) .GT. (50) )IFLAG = 10                                 PLS05640
800   CONTINUE                                                          PLS05650
      IF( IFLAG .LT. 1)GOTO 900                                         PLS05660
      WRITE(6,2030)                                                     PLS05670
      STOP                                                              PLS05680
900   RETURN                                                            PLS05690
2000  FORMAT(' MAXA = ',I5, ' MAXB = ',I5)                              PLS05700
2010  FORMAT(' MINA = ',I5,' MINB = ',I5)                               PLS05710
2020  FORMAT(' JMAX = ',I5,' NCHG = ',I5)                               PLS05720
2030  FORMAT(' ***PGM ABORT IN SUBR DELTA.  NSUB GT (15) ')             PLS05730
2040  FORMAT(' ***PGM ABORT IN SUBR DELTA.  JMAX GT (10) ')             PLS05740
      END                                                               PLS05750
C                                                                       PLS05760
      SUBROUTINE VOID(NDIV,DTDP,RHO1,RHO2,EBAR,EPS)                     PLS05770
      ZNDIV = NDIV                                                      PLS05780
      DELR = (RHO2 - RHO1 ) /ZNDIV                                      PLS05790
      ROLD = RHO1                                                       PLS05800
      FOLD = RHO1*EFUNC(RHO1, DTDP, EBAR)                               PLS05810
      SUM = 0.0                                                         PLS05820
      DO 100 I=1,NDIV                                                   PLS05830
      RNEW = ROLD + DELR                                                PLS05840
      FNEW = RNEW * EFUNC(RNEW, DTDP, EBAR)                             PLS05850
      FINT = 0.5*DELR*(FNEW + FOLD)                                     PLS05860
      SUM = SUM + FINT                                                  PLS05870
      FOLD = FNEW                                                       PLS05880
      ROLD = RNEW                                                       PLS05890
100   CONTINUE                                                          PLS05900
      VTOT = RHO2*RHO2 - RHO1*RHO1                                      PLS05910
      EPS = SUM                                                         PLS05920
      EPS = 2.0*EPS/VTOT                                                PLS05930
      RETURN                                                            PLS05940
      END                                                               PLS05950
C                                                                       PLS05960
      FUNCTION EFUNC(R, DTDP, EBAR)                                     PLS05970
      PI = 2.0*ARSIN(1.0)                                               PLS05980
      A1 = 0.3463                                                       PLS05990
      A2 = 0.4273                                                       PLS06000
      A3 = 2.4509                                                       PLS06010
      A4 = 2.2011                                                       PLS06020
      X = 0.5*DTDP*(1.0-R)                                              PLS06030
      IF( X .LT. 0.25) GOTO 100                                         PLS06040
      YY = COS( (A3*X-A4)*PI )                                          PLS06050
      YY = A1*YY/EXP(A2*X)                                              PLS06060
      EFUNC = (1.0-EBAR)*YY + EBAR                                      PLS06070
      GOTO 1000                                                         PLS06080
100   CONTINUE                                                          PLS06090
C  THIS SECTION FOR 'WALL' REGION                                       PLS06100
      YY = 7.0*X*X/9.0                                                  PLS06110
      YY = 4.5*(X-YY)                                                   PLS06120
      YY = (1.0-EBAR)*YY                                                PLS06130
      EFUNC = 1.0-YY                                                    PLS06140
1000  RETURN                                                            PLS06150
      END                                                               PLS06160
C                                                                       PLS06170
C                                                                       PLS06180
      SUBROUTINE MIX1(NA,NB)                                            PLS06190
C  THIS SUBROUTINE DETERMINES WEIGHT FACTORS FOR                        PLS06200
C  MIXING AT ARNOLDS INLETS                                             PLS06210
      COMMON /TWO/ Q(20),A(20),B(20)                                    PLS06220
      N = NA+NB                                                         PLS06230
      IF(NA .LE. NB) GOTO 200                                           PLS06240
C  THIS SECTION FOR NA G1 NB                                            PLS06250
C  NEED WEIGHTS FOR ODD NUMBERED SEGMENTS                               PLS06260
      W(N) = 0.0                                                        PLS06270
      W(1) = 1.0                                                        PLS06280
      N2 = N-2                                                          PLS06290
      DO 10 I=3,N2,2                                                    PLS06300
      I1 = N2 - I + 3                                                   PLS06310
      W(I1) = ( Q(I1+1) - (1.0-W(I1+2))*Q(I1+2) )/Q(I1)                 PLS06320
10    CONTINUE                                                          PLS06330
      GOTO 1000                                                         PLS06340
200   CONTINUE                                                          PLS06350
C  THIS SECTION FOR NA = NB                                             PLS06360
C  NEED WEIGHTS FOR EVEN NUMBERED SEGMENTS                              PLS06370
      W(N) = 0.0                                                        PLS06380
      N2 = N-2                                                          PLS06390
      DO 300 I=2,N2,2                                                   PLS06400
```

```
      I1 = 2-I+N2                                                       PLS06410
      W(I1) = ( Q(I1+1) - (1.0-W(I1+2))*Q(I1+2) )/Q(I1)                 PLS06420
  300 CONTINUE                                                          PLS06430
 1000 CONTINUE                                                          PLS06440
      RETURN                                                            PLS06450
      END                                                               PLS06460
```

Steady-state Heat Dispersion

General program flow follows that for steady-state mass dispersion, but with added steps of numerical integration along the length of each half-cell (subroutine CELLIN) between mixing calculations. As for mass dispersion, two versions of subroutine ANN are given. Other programming details are commented in the listing.

```
C  PROGRAM BASE 'TEMPV3 FORTRAN'                                        DUM00010
C                                                                       DUM00020
C  ------------------------------------------------------               DUM00030
C  THIS RUN FOR DATA OF LEROU AND FROMENT--CYLINDERS                    DUM00040
C  ------------------------------------------------------               DUM00050
C                                                                       DUM00060
C  LAST UPDATE/USE ON 28 JUNE 85                                        DUM00070
       DIMENSION EPS(100),AXS(100)                                      DUM00080
       DIMENSION TIN(100)                                               DUM00090
       DIMENSION Q(100),B(100),A(100),YEL(100)                          DUM00100
       DIMENSION W(100),C(100),T(100)                                   DUM00110
       DIMENSION BA(100),SB(100)                                        DUM00120
       COMMON /ONE/ TOLD(100), HR(100), LASTOR                          DUM00130
       COMMON /RS/ HP,RR,DT,DP,CP,TBALL,G,WEIGHT,ISHAPE,APELL           DUM00140
       DATA TIN /100*20.5/                                              DUM00150
       DATA NLONG,NPRINT /49,0/                                         DUM00160
C  THIS PROGRAM CALCULATES FLOWS AND TEMPERATURES GIVEN                 DUM00170
C  ANNULUS DIMENSIONS.                                                  DUM00180
C                                                                       DUM00190
       DATA C /100*0.0/                                                 DUM00200
       DATA R /100*0.0/                                                 DUM00210
C  NOTE--THE VARIABLE 'ISHAPE' DENOTES SHAPE OF PARTICLES               DUM00220
       DIMENSION PSIP(5),PSIW(5)                                        DUM00230
       DATA PSIP / 1.0 , 1.0, 3*1.0 /                                   DUM00240
       DATA PSIW /1.0, 1.0, 3*1.0/                                      DUM00250
C         (EFFECT HEAT TRANSFER CASES)                                  DUM00260
C         IF ISHAPE = 1 ==> SPHERES                                     DUM00270
C                   = 2 ==> CYLINDERS                                   DUM00280
C  IT IS THE SUBSCRIPT OF THE 'SHAPE FACTOR' VECTOR, PSI                DUM00290
C         TO BE USED IN THE J-FACTOR ANALOGY. . .                       DUM00300
C            H = CONST * PSI * H(SPHERE)                                DUM00310
C         PSIP==PELLET H; PSIW==WALL H                                  DUM00320
       ISHAPE = 2                                                       DUM00330
C                                                                       DUM00340
C*****************                                                      DUM00350
       WRITE(6,2370)                                                    DUM00360
       DI = 3.6                                                         DUM00370
       ZDP = 0.26                                                       DUM00380
       ZLP = ZDP                                                        DUM00390
       DP = ZDP*ZDP + ZLP*ZLP                                           DUM00400
       DP = SQRT(0.5*DP)                                                DUM00410
C  DON'T FORGET THAT ZLP=ZDP FOR SPHERICAL PELLETS                      DUM00420
C  ALSO, FORM OF SURF AREA/VOL (APELL) CHANGES WITH SHAPE...            DUM00430
       APELL = 6.0/ZDP                                                  DUM00440
       DTDP = DT/DP                                                     DUM00450
       DO 10 I=1,100                                                    DUM00460
10     W(I) = 20.0                                                      DUM00470
C  NOW, TRY ASSIGNING NO. CELLS BASED ON CORRELATION...                 DUM00480
       Z = DTDP/0.816 + 0.5                                             DUM00490
       N = Z                                                            DUM00500
       Z = N                                                            DUM00510
       Z = 0.5*Z                                                        DUM00520
       NB = Z                                                           DUM00530
       NA = N-NB                                                        DUM00540
C  RESTRICT TO EVEN NO. SEGMENTS                                        DUM00550
       IF(NA .GT. NB)NB = NA                                            DUM00560
       N = NA+NB                                                        DUM00570
       WRITE(6,2020)DTDP,N,NA,NB                                        DUM00580
C  SIZE RADII                                                           DUM00590
C  SET UP TO DO INCREASING EA'S...                                      DUM00600
C  SIZE EVENLY SPACED RADII                                             DUM00610
       ZN = N/2                                                         DUM00620
       DELR = 1.0/ZN                                                    DUM00630
       R(2) = DELR                                                      DUM00640
       DO 80 I=4,N,2                                                    DUM00650
       R(I) = R(I-2) + DELR                                             DUM00660
80     CONTINUE                                                         DUM00670
C  DETERMINE EPS FOR EACH SEGMENT...                                    DUM00680
       EBAR = 0.32                                                      DUM00690
C  VOID FRACTION OF FIRST SEGMENT                                       DUM00700
       CALL VOID(DTDP,0.0,R(2),EBAR,E1)                                 DUM00710
       I=2                                                              DUM00720
       WRITE(6,2010)I,E1                                                DUM00730
100    CONTINUE                                                         DUM00740
       EPS(1) = E1                                                      DUM00750
       EPS(2) = E1                                                      DUM00760
       XI = R(2)*R(2)                                                   DUM00770
       AXS(1) = XI                                                      DUM00780
       AXS(2) = XI                                                      DUM00790
       BA(1) = (1.0-E1)*XI                                              DUM00800
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```
      RA(1) = SQRT( RA(1) )                                              00E00810
      RB(1) = E1*IX                                                      00M00820
      RB(1) = SQRT( RB(1) )                                              00P00830
      RA(2) = R(2)                                                       00M00840
      RB(2) = R(2)                                                       00E00850
      MAX = N-1                                                          00M00860
      DO 120 I=3,MAX,2                                                   00E00870
C  VOID FRACTIONS OF RADIAL CELLS BASED ON CORRELATION                   00E00880
      RHO2 = R(I+1)                                                      00E00890
      RHO1 = R(I-1)                                                      00M00900
      CALL VOID(UTDP,RHO1,RHO2,RBAR,EBAR)                                00M00910
      IW = I+1                                                           00M00920
      WRITE(6,2010)IW,EBAT                                               00E00930
      IX = R(I+1)*R(I+1) - R(I-1)*E(I-1)                                 00M00940
      AXS(I) = IX                                                        00M00950
      AXS(IW) = IX                                                       00M00960
      EPS(I) = EBAT                                                      00M00970
      EPS(IW) = EBAT                                                     00M00980
      RA(I) = (1.0-EBAT)*IX                                              00M00990
      RA(I) = R(I-1)*R(I-1) + RA(I)                                      00E01000
      RA(I) = SQRT( RA(I) )                                              00M01010
      RB(I) = EBAT * IX                                                  00M01020
      RB(I) = R(I-1)*R(I-1) + RB(I)                                      00M01030
      RB(I) = SQRT( RB(I) )                                              00M01040
      RA(IW) = R(IW)                                                     00M01050
      RB(IW) = R(IW)                                                     00M01060
120   CONTINUE                                                           00M01070
      MAX = N-1                                                          00M01080
      WRITE(6,2150)                                                      00M01090
      WRITE(6,2160) (RA(I),R(I+1),I=1,MAX,2)                             00M01100
      WRITE(6,2160) (RB(I),R(I+1),I=1,MAX,2)                             00M01110
      CALL ANR(RA,RB,Q,R,A,E1,E2,RA,RB)                                  00M01120
      CALL RIXI(RA,RB,Q,N)                                               00M01130
C  *****DON'T FORGET HEAT I-FEB GOOGIES*****                            00E01140
C  HEAT I-FEB DATA GOES HERE                                           00M01150
C  --- C.G.S. UNITS---                                                 00M01160
C                                                                      00E01170
CCC   TIB = 30.0                                                        00M01180
      DO 1 I=1,100                                                       00E01190
1     TOLD(I) = TIN(I)                                                   00M01200
      TBALL = 100.0                                                      00E01210
      CP = 0.25                                                          00M01220
C  NOTE--USING SYMBOL 'G' TO SIGNIFY MASS FLOW RATE                     00E01230
C    (G/SEC) AND *NOT* MASS FLUX (G/SEC-CM**2) !!!!                     00M01240
C  -----GDOT==>MASS FLUX; GBASE==>BASE CASE MASS FLUX                   00M01250
C  ---------- INTERSTITIAL VALUES ------------------                    00M01260
      IX = 0.4*1600.0                                                    00M01270
      GBASE = 274.0/IX                                                   00E01280
      GWALL =  7.17 * 454.0 / 3600.0                                     00M01290
      WW = 1.80                                                          00E01300
      G = WW                                                             00E01310
      IX = 3.1416*0.25*DT*DT*E1                                          00M01320
      GDOT = G/IX                                                        00M01330
C  TRY BY CORRELATION FOR HF AND HB. . .                                00E01340
C  INCLUDE TEMP DEPENDENCE OF DENSITY FOR VELOCITY PURPOSES             00M01350
      TBASE = 60.0+273.15                                                00E01360
      TEMP = (TIN(1)+TWALL)/2. + 273.15                                  00M01370
      BP = 1.08-3 * SQRT( TEMP*GDOT**0.6/(GBASE * TBASE * DP) )          00M01380
      BP = BP*1.0                                                        00M01390
CCC   HW = 2.40E-3                                                       00E01400
      HW = 2.08E-3*( GDOT/GBASE )**0.8                                   00M01410
      WRIGHT = 0.10                                                      00M01420
      WRITE(6,2360) BW,BP,WEIGHT,TEMP                                    00E01430
      STUFF = G * CP * DTDP                                              00M01440
      STOFF = 4.0*SQRT(2.0/3.0) / STUFF                                  00M01450
      STUFF = STUFF/Q(N)                                                 00M01460
      DO 200 I=1,N                                                       00E01470
      VEL(I) = E1*Q(I)/A(I)                                              00M01480
200   CONTINUE                                                           00M01490
      WRITE(6,2050)                                                      00M01500
      DO 300 I=2,N,2                                                     00M01510
      J = I-1                                                            00M01520
      WRITE(6,2060)I,A(I),Q(I),VEL(I),J,A(J),Q(J),VEI(J)                 00M01530
300   CONTINUE                                                           00E01540
      WRITE(6,2070) E1,E2                                                00E01550
      WRITE(6,2150)                                                      00M01560
CCC   WRITE(6,2160) (B(I),I=1,N)                                         00E01570
      N = NA + NB                                                        00M01580
C  INITIALIZE PROFILE.                                                  00E01590
      DO 420 I=1,N                                                       00E01600
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      T(I) = TIN(I)                                                     DUM01610
420   CONTINUE                                                          DUM01620
C  NOW, CALC TEMPERATURES...                                           DUM01630
CCC   WRITE(6,2230)                                                     DUM01640
      KOUNT = 0                                                         DUM01650
500   KOUNT = KOUNT+1                                                  DUM01660
      WRITE(6,2240)KOUNT                                                DUM01670
      IF(KOUNT .GT. NLONG)GOTO 1000                                     DUM01680
C  RECALC FLOW DISTRIB BASED ON T PROFILE                               DUM01690
C  USE LAST CELL'S TEMP TO CALC HW                                      DUM01700
CCC   HW = HWALL( T(8), 238.0, DP)                                      DUM01710
CCC   BZ = 238.0                                                        DUM01720
CCC   BP = BPELL( T(1), BZ, DP)                                         DUM01730
CCC   ALP = STOFF*BW                                                    DUM01740
CCC   ALP = 0.0                                                         DUM01750
CCC   WRITE(6,2310)BP,HW                                                DUM01760
C  ---------------------------------------------------------------------DUM01770
C  NUMERICAL INTEGRATION ALONG THE LENGTH OF EACH HALF-CELL             DUM01780
CCC   WRITE(6,2320)                                                     DUM01790
CCC   WRITE(6,2400) (I,T(I),I=1,N)                                      DUM01800
      CALL CELLIN(1,N,Q,T,RA,RB,R,EPS,AXS)                              DUM01810
      WRITE(6,2330)                                                     DUM01820
      WRITE(6,2400) (I,T(I),I=1,N)                                      DUM01830
      CALL MIX2(0,NA,NB,Q,R,T,TWALL,0.0)                                DUM01840
CCC   WRITE(6,2340)                                                     DUM01850
CCC   WRITE(6,2400) (I,T(I),I=1,N)                                      DUM01860
      CALL CELLIN(0,N,Q,T,RA,RB,R,EPS,AXS)                              DUM01870
      WRITE(6,2350)                                                     DUM01880
      WRITE(6,2400) (I,T(I),I=1,N)                                      DUM01890
C  CALC AVG TEMPS AND WRITE RESULTS                                     DUM01900
C        ASSUME EVEN NO. RADIAL DIVISIONS                               DUM01910
      TAVAR = 0.0                                                       DUM01920
      TSAR = 0.0                                                        DUM01930
      DO 520 I=2,N,2                                                    DUM01940
      J=I-1                                                             DUM01950
      TAVAR = TAVAR + Q(I)*T(I)                                         DUM01960
      TSAR = TSAR + Q(J)*T(J)                                           DUM01970
CCC   WRITE(6,2250) I,Q(I),T(I),J,Q(J),T(J)                             DUM01980
520   CONTINUE                                                          DUM01990
      WRITE(6,2300) TAVAR,TSAR                                          DUM02000
710   CONTINUE                                                          DUM02010
C  CALC A-INLETS...                                                     DUM02020
      CALL MIX2(1,NA,NB,Q,R,T,TWALL,0.0)                                DUM02030
      GOTO 500                                                          DUM02040
1000  CONTINUE                                                          DUM02050
C  FORMATS. . .                                                         DUM02060
2010  FORMAT(' I =',I4,'   EPS = ',E11.4)                               DUM02070
2015  FORMAT(' ALPHA =',E11.4)                                          DUM02080
2020  FORMAT(' DTEP = ',E11.4,'  N =',I3,'  NA =',I3,'  NB =',I3)       DUM02090
2030  FORMAT(' D1/B =',E11.4)                                           DUM02100
2040  FORMAT(' F = ',E11.4)                                             DUM02110
2050  FORMAT(20X,'A',33X,'B',/,2X,40('-'),2X,40('-'),/,                 DUM02120
     1 2(2X,'I',7X,'A',11X,'F',9X,'VEL  ',5X),/,                        DUM02130
     2 1X,2('----',2X,3('----------',2X)))                              DUM02140
2060  FORMAT(1X,2(I3,2X,3(E10.4,2X)))                                   DUM02150
2070  FORMAT(' Z1 = ',E11.4,'  Z2 = ',E11.4)                            DUM02160
2150  FORMAT(' RADII...')                                               DUM02170
2160  FORMAT(5(2X,E11.4))                                               DUM02180
2170  FORMAT(' MIXING WEIGHT FACTORS. . .')                             DUM02190
2230  FORMAT(9X,'A',30X,'B',/,2(2X,29('-')),/,                          DUM02200
     1 2X,2(1X,'I',8X,'G',7X,3X,'  T  ',4X),/,                          DUM02210
     2 2X,2('---',2X,'----------',2X,'----------',2X))                  DUM02220
C23456789.123456789.123456789.123456789.123456789.123456789.           DUM02230
2240  FORMAT(' CELL NO ',I5)                                            DUM02240
2250  FORMAT(2X,2(I3,2X,E11.4,2X,E11.4,2X))                             DUM02250
2260  FORMAT(' HA = ',E11.4,'   EBBD = ',E11.4)                         DUM02260
2270  FORMAT(' CALC. INVALID VOID FRACT.  PGM ABORTED ')                DUM02270
2290  FORMAT(' F =',E11.4,' SUM =',E11.4,' EPS1 =',E11.4)               DUM02280
2300  FORMAT(' AVG TEMPS ',2X,E11.4,10X,E11.4)                          DUM02290
2310  FORMAT(' ---BP = ',E11.4,'  HW = ',E11.4)                         DUM02300
2320  FORMAT(' A INLETS...')                                            DUM02310
2330  FORMAT(' A OUTLETS...')                                           DUM02320
2340  FORMAT(' B INLETS...')                                            DUM02330
2350  FORMAT(' B OUTLETS...')                                           DUM02340
2360  FORMAT(' DW =',E11.4,'   BP =',E11.4,'   WEIGHT =',E11.4,         DUM02350
     * '  T(DENSITY,K)=',E11.4)                                         DUM02360
2370  FORMAT(5(' *'),'TEMPV3',5(' *'))                                  DUM02370
2400  FORMAT( 8 (I8,2X,E11.4) )                                         DUM02380
      STOP                                                              DUM02390
      END                                                               DUM02400
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C                                                                       DUM02410
C                                                                       DUM02420
      SOBROUTINE ANN(NA,NB,Q,R,A,Z1,Z2,BA,BB)                           DUM02430
      DIMENSION BA(100),BB(100)                                         DUM02440
      DIMENSION Q(100),R(100),BH(100),A(100)                            DUM02450
C  CALC  HYDRAULIC RADII, AND AREAS                                     DUM02460
      N = NA + NB                                                       DUM02470
C  A HALF-CELL                                                          DUM02480
      DO 10 I=2,N,2                                                     DUM02490
      BH(I) = R(I) - BA(I-1)                                            DUM02500
      A(I) = R(I)*R(I) - BA(I-1)*BA(I-1)                                DUM02510
10    CONTINUE                                                          DUM02520
C  B HALF-CELL                                                          DUM02530
      BH(1) = BB(1)                                                     DUM02540
      A(1) = BB(1)*BB(1)                                                DUM02550
      MAX = N-1                                                         DUM02560
      DO 20 I=3,MAX,2                                                   DUM02570
      BH(I) = BB(I) - R(I-1)                                            DUM02580
      A(I) = BB(I)*BB(I) - R(I-1)*R(I-1)                                DUM02590
20    CONTINUE                                                          DUM02600
C  NOW, DETERMINE FLOWS AND POROSITIES OF A AND B SEGS                  DUM02610
C  DEPENDS ON NA AND NB                                                 DUM02620
      IF(NA .LE. NB) GOTO 500                                           DUM02630
C  THIS SECTON FOR NA GT NB                                             DUM02640
C  FLOW DISTRIBUTION AND POROSITY                                       DUM02650
      Z1 = 0.0                                                          DUM02660
      SUM = 0.0                                                         DUM02670
      DO 100 I=1,N,2                                                    DUM02680
      Z1 = Z1 + A(I)                                                    DUM02690
100   SUM = SUM + A(I)*SQRT(BH(I))                                      DUM02700
      DO 110 I=1,N,2                                                    DUM02710
      Q(I) = A(I)*SQRT(BH(I))/SUM                                       DUM02720
110   CONTINUE                                                          DUM02730
C  B SEGMENT                                                            DUM02740
      Z2 = 0.0                                                          DUM02750
      SUM = 0.0                                                         DUM02760
      N1 = N-1                                                          DUM02770
      DO 120 I=2,N1,2                                                   DUM02780
      Z2 = Z2+A(I)                                                      DUM02790
120   CONTINUE                                                          DUM02800
      XX = A(N-1)*SQRT( BH(N-1) )                                       DUM02810
      YY = A(N-3) *SQRT( BH(N-3) )                                      DUM02820
      Q(N-1) = Q(N) + Q(N-2)*XX/(XX+YY)                                 DUM02830
      XX = A(2)*SQRT(BH(2))                                             DUM02840
      YY = A(4)*SQRT(BH(4))                                             DUM02850
      Q(2) = Q(1) + Q(3)*XX/(XX+YY)                                     DUM02860
      MAX = N-3                                                         DUM02870
C  DON'T NEED FOLLOWING IF N .LE. 5                                     DUM02880
      IF(N .LE. 5)GOTO 1000                                             DUM02890
      DO 130 I=4,MAX,2                                                  DUM02900
      XX = A(I)*SQRT(BH(I))                                             DUM02910
      YY = A(I-2)*SQRT(BH(I-2))                                         DUM02920
      ZZ = A(I+2)*SQRT(BH(I+2))                                         DUM02930
      Q(I) = Q(I-1)*XX/(XX+YY) + Q(I+1)*XX/(XX+ZZ)                      DUM02940
130   CONTINUE                                                          DUM02950
      GOTO 1000                                                         DUM02960
500   CONTINUE                                                          DUM02970
C  THIS SECTION FOR NA=NB                                               DUM02980
C  FLOW DISTRIBUTION AND POROSITY                                       DUM02990
C  A-SEGMENT                                                            DUM03000
      SUM = 0.0                                                         DUM03010
      Z1 = 0.0                                                          DUM03020
      DO 510 I=2,N,2                                                    DUM03030
      Z1 = Z1 + A(I)                                                    DUM03040
510   SUM = SUM + A(I)*SQRT(BH(I))                                      DUM03050
      DO 520 I=2,N,2                                                    DUM03060
      Q(I) = A(I)*SQRT(BH(I))/SUM                                       DUM03070
520   CONTINUE                                                          DUM03080
C  B-SEG                                                                DUM03090
      Z2 = 0.0                                                          DUM03100
      SUM = 0.0                                                         DUM03110
      N1 = N-1                                                          DUM03120
      DO 530 I=1,N1,2                                                   DUM03130
      Z2 = Z2+A(I)                                                      DUM03140
530   CONTINUE                                                          DUM03150
C  TRY SUBDIVIDING BASED ON SQRT(RH)                                    DUM03160
C        --INSTEAD OF A*SQRT(RH)                                        DUM03170
      XX = A(N-1)*SQRT(RH(N-1))                                         DUM03180
      YY = A(N-3) *SQRT(RH(N-3))                                        DUM03190
      Q(N-1) = Q(N) + Q(N-2)*XX/(XX+YY)                                 DUM03200
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      RX = A(I)*SQRT(RH(I))                                              COMM3210
      TT = A(J)*SQRT(RH(J))                                              COMM3220
      Q(I) = Q(2)*TT/(TT+RX)                                             COMM3230
      NA2 = N-3                                                          COMM3240
C  DON'T NEED FOLLOWINGIF N .LE. 4                                       COMM3250
      IF( N .LE. 4)GOTO 1000                                             COMM3260
      DO 500 I=3,NA2,2                                                   COMM3270
      RX = A(I)*SQRT(RH(I))                                              COMM3280
      TT = A(I-2)*SQRT(RH(I-2))                                          COMM3290
      ZZ = A(I+2)*SQRT(RH(I+2))                                          COMM3300
      Q(I) = Q(I-1)*RX/(TT+RX) + Q(I+1)*RX/(RX+ZZ)                       COMM3310
500   CONTINUE                                                           COMM3320
1000  RETURN                                                             COMM3330
      END                                                                COMM3340
C                                                                        COM03350
C                                                                        COM03360
C                                                                        COM03370
      SUBROUTINE VOID(DTUP,RHO1,RHO2,EBAR,EPS)                           COM03380
      PI = 2.0*ARSIN(1.0)                                                COMM3390
      A1 = 0.3463                                                        COM03400
      A2 = 0.4273                                                        COM03410
      A3 = 2.8509                                                        COM03420
      A4 = 2.2011                                                        COMM3430
      ALP = 0.5*DTUP* A2                                                 COMM3440
      B = (A3 - A4)*PI*DTUP/2.0                                          COMM3450
      C = A3 * PI * DTUP / 2.0                                           COM03460
      A = A1 * (1.0-EBAR) * EXP(-1.0*ALP)                                COMM3470
CCC   WRITE(6,2000)A,ALP,B,C,DTUP                                        COMM3480
      R2 = RHO2                                                          COMM3490
      R1 = RHO1                                                          COM03500
      VAZE = 0.0                                                         COMM3510
      V = 0.0                                                            COM03520
      TEST = 1.0-0.5/DTUP                                                COM03530
      IF(RHO2 .LE. TEST)GOTO 100                                         COM03540
C  THIS SECTION TREATS OUTERMOST ANNULUS.  VOID BETWEEN                  COM03550
C  WALL AND 0.25DP HAS DIFFERENT FUNCTION.....                           COM03560
      VAZE = 0.5 - 0.24479*(1.0-EBAR)                                    COM03570
      VADD = VADD*DTUP - 0.125                                           COM03580
      VAZD = VADD/(DTUP*DTUP)                                            COM03590
      R2 = TEST                                                          COM03600
      IF(RHO1 .GE. TEST)GOTO 200                                         COM03610
100   CONTINUE                                                           COM03620
      V = 0.5*EBAR*(R2*R2-R1*R1)                                         COMM3630
      ARG = B-C*R2                                                       COM03640
      F2 = ALP*COS(ARG) - C*SIN(ARG)                                     COM03650
      F2 = F2 * EXP( ALP*R2 )                                            COM03660
      ARG = B-C*R1                                                       COM03670
      F1 = ALP*COS(ARG) - C*SIN(ARG)                                     COM03680
      F1 = F1*EXP( ALP*R1 )                                              COM03690
      V = V + (F2-F1)*A/(ALP*ALP + C*C)                                  COMM3700
200   VVCIU = 2.0*(V + VADD)                                             COM03710
      VIOI = RHO2*RHO2 - RHO1*RHO1                                       COM03720
      EPS = VVOID/VIOI                                                   COM03730
C2000 FORMAT(' A, ALP, B, C, DTUP . . . ',/,8(2X,E11.4) )                COM03740
      RETURN                                                             COMM3750
      END                                                                COM03760
C                                                                        COMM3770
C                                                                        COM03780
      SUBROUTINE MIX1(NA,NB,Q, W)                                        COM03790
C  THIS SUBROUTINE DETERMINES WEIGHT FACTORS FOR                         COM03800
C  MIXING AT ANNULUS INLETS                                              COM03810
      DIMENSION Q(100),W(100)                                            COM03820
      N = NA+NB                                                          COMM3830
      IF(NA .LE. NB) GOTO 200                                            COM03840
C  THIS SECTION FOR NA GT NB                                             COMM3850
C  NEED WEIGHTS FOR ODD NUMBERED SEGMENTS                                COMM3860
      W(N) = 0.0                                                         COM03870
      W(1) = 1.0                                                         COM03880
      N2 = N-2                                                           COM03890
      DO 1U I=3,N2,2                                                     COMM3900
      I1 = N2 - I + 3                                                    COM03910
      W(I1) = ( Q(I1+1) - (1.0-W(I1+2))*Q(I1+2) )/Q(I1)                  COMM3920
1U    CONTINUE                                                           COM03930
      GOTO 1000                                                          COMM3940
200   CONTINUE                                                           COMM3950
C  THIS SECTION FOR NA = NB                                              COMM3960
C  NEED WEIGHTS FOR EVEN NUMBERED SEGMENTS                               COM03970
      W(N) = 0.0                                                         COM03980
      N2 = N-2                                                           COM03990
      DO 3UU I=2,N2,2                                                    COM04000
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      I1 = 2-I+N2                                                       COM04010
      W(I1) = ( Q(I1+1) - (1.0-W(I1+2)) *Q(I1+2) )/Q(I1)                COM04020
  300 CONTINUE                                                          COM04030
 1000 CONTINUE                                                          COM04040
      RETURN                                                            COM04050
      END                                                               COM04060
      SUBROUTINE MIX2(ITRANS,NA,NB,Q,W,C,TWALL,ALP)                     COM04070
      DIMENSION W(100),Q(100),C(100)                                    COM04080
C  THIS SUBROUTINE DETERMINES ARRHUIUS INLET CONCENTRATIONS             COM04090
C  ITRANS=0==>A TO B TRANSITION                                         COM04100
C         =1==>B TO A TRANSITION                                        COM04110
      N = NA+NB                                                         COM04120
C  ASSUME NA = NB                                                       COM04130
C  NOTE--USING C ARRAY TO HOLD T-VALUES                                 COM04140
  500 CONTINUE                                                          COM04150
C  THIS SECTION FOR NA=NB                                             COM04160
      IF(ITRANS .NE. 0)GOTO 700                                         COM04170
C  A TO B TRANS                                                         COM04180
C  B'S ODD NUMBERED SUBSCRIPTS                                        COM04190
      C(1) = C(2)                                                       COM04200
      N1 = N-1                                                          COM04210
      DO 600 I=3,N1,2                                                   COM04220
      C(I) = (1.0-W(I+1))*Q(I+1)*C(I+1)                                 COM04230
      C(I) = C(I) + W(I-1)*Q(I-1)*C(I-1)                                COM04240
      C(I) = C(I) / Q(I)                                                COM04250
  600 CONTINUE                                                          COM04260
      RETURN                                                            COM04270
  700 CONTINUE                                                          COM04280
C  B TO A TRANSITION                                                    COM04290
C  A'S EVEN NUMBERED SUBSCRIPTS                                       COM04300
C  USE HEAT BAL TO CALC OUTERMOST TEMP                                COM04310
CCC   XX = EXP( -1.0 * ALP )                                           COM04320
CCC   C(N) = TWALL + ( C(N-1)-TWALL )*XX                               COM04330
      C(N) = C(N-1)                                                     COM04340
      N2 = N-2                                                          COM04350
      DO 800 I=2,N2,2                                                   COM04360
      C(I) = W(I)*C(I+1) + (1.0-W(I))*C(I-1)                            COM04370
  800 CONTINUE                                                          COM04380
      RETURN                                                            COM04390
      END                                                               COM04400
      FUNCTION HWALL(T,BE,DP)                                           COM04410
C  ------ T IS IN DEGREES CELSIUS ------                                COM04420
C  USE Y & W CORRELATION                                              COM04430
      FACTOR = 0.18 * RE**0.80                                          COM04440
      ZKAIR = 0.1663*(T+273.15) + 12.893                                COM04450
      ZKAIR =ZKAIR*1.0E-6                                               COM04460
      HWALL = 0.1*FACTOR * ZKAIR/DP                                     COM04470
      RETURN                                                            COM04480
      END                                                               COM04490
C                                                                       COM04500
      FUNCTION HPELL(T,BE,DP)                                           COM04510
C  USE B.S.L. CORREL..                                                COM04520
      ZKAIR = 0.1663*(T+273.15) + 12.893                                COM04530
      ZKAIR = ZKAIR * 1.0E-6                                            COM04540
      CEND = 4.8385E-5                                                  COM04550
CCC   PR = CPMU/ZKAIR                                                   COM04560
      PR = 0.66                                                         COM04570
      FACTOR = PR**0.33333                                              COM04580
      FACTOR = 2.0 + 0.6*SQRT(BE)*FACTOR                                COM04590
      HPELL = FACTOR * ZKAIR/DP                                         COM04600
      RETURN                                                            COM04610
      END                                                               COM04620
      SUBROUTINE CELLIN(ITRANS,N,Q,T,BA,BB,R,EPS,AXS)                   COM04630
      DIMENSION EPS(100),AXS(100), T(100),Q(100)                        COM04640
      DIMENSION BA(100),BB(100),R(100)                                  COM04650
      COMMON /BLK/ HP,HW,DT,DP,CP,TWALL,G,WEIGHT,ISHAPE,APELL           COM04660
      DATA ISHAPE /1.0, 0.6667, 3*1.0/                                  COM04670
C                                                                       COM04680
C  ITRANS =EQ. 1==>WE'RE IN A                                           COM04690
C         =EQ. 0==>WE'RE IN B                                           COM04700
C  DEFINE NUMERICAL INTEGRATION PARAMETERS                            COM04710
      DIV = 1.0                                                         COM04720
      PI = 3.1416                                                       COM04730
      DZ = 0.816*DP/DIV                                                 COM04740
      IZMAX = DIV                                                       COM04750
      IF(ITRANS .EQ. 0) GOTO 500                                        COM04760
C  THIS SECTION FOR A-HALF-CELL                                         COM04770
C  ALREADY HAVE INLET TEMPS...                                        COM04780
      DO 100 IZ=1,IZMAX                                                 COM04790
                                                                        COM04800
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C  CALC SOLID TEMPS AS AVG OF SURROUNDING FLUIDS                  DUM04810
      T(1) = T(2)                                                 DUM04820
      MAX = N-1                                                   DUM04830
      DO 50 I=3,MAX,2                                             DUM04840
      T(I) = 0.5*( T(I+1) + T(I-1) )                              DUM04850
50    CONTINUE                                                    DUM04860
C  NOW FLUID TEMPS                                                DUM04870
C  WALL AND PLUG 2 DIFFERENT                                      DUM04880
      DTDZ = HX*PI*DI*(TWALL-T(N))                                DUM04890
      AP = (1.0-EPS(N))*AXS(N)                                    DUM04900
      AP = ISHAPE(ISHAPE)*0.25*APELL*PI*DI*DI*AP                  DUM04910
      DTDZ = DTDZ - HP*AP*( T(N)-T(N-1) )                         DUM04920
      XI = Q(N)*CP*G                                              DUM04930
      T(N) = T(N) + DZ*DTDZ/XI                                    DUM04940
      XI = Q(2)*CP*G                                              DUM04950
      AP = (1.0-EPS(2))*AXS(2)                                    DUM04960
      AP = ISHAPE(ISHAPE)*0.25*APELL*PI*DI*DI*AP                  DUM04970
      DTDZ = HP*AP*( T(3)-T(2) )                                  DUM04980
      T(2) = T(2) + DZ*DTDZ/XI                                    DUM04990
      I=2                                                         DUM05000
      MAX = N-2                                                   DUM05010
      DO 60 I=4,MAX,2                                             DUM05020
      XI = Q(I)*CP*G                                              DUM05030
      APTOP = ISHAPE(ISHAPE)*(1.0-EPS(I+1))*AXS(I+1)              DUM05040
      APBOT = ISHAPE(ISHAPE)*(1.0-EPS(I-1))*AXS(I-1)              DUM05050
      DTDZ = APTOP*( T(I+1)-T(I) ) - APBOT*( T(I)-T(I-1) )        DUM05060
      DTDZ = DTDZ*HP*0.25*APELL*PI*DI*DI/XI                       DUM05070
      T(I) = T(I) + DZ*DTDZ                                       DUM05080
60    CONTINUE                                                    DUM05090
100   CONTINUE                                                    DUM05100
C  NOW, HAVE OUTLET FLOID TEMPS, BUT                              DUM05110
C     MUST CALC NEW SOLID TEMPS.                                  DUM05120
      T(1) = T(2)                                                 DUM05130
      MAX = N-1                                                   DUM05140
      DO 110 I=3,MAX,2                                            DUM05150
      T(I) = 0.5*(T(I+1)+T(I-1))                                  DUM05160
110   CONTINUE                                                    DUM05170
      GOTO 1000                                                   DUM05180
C  THIS SECTION FOR B-HALF-CELL                                   DUM05190
500   CONTINUE                                                    DUM05200
      DO 600 IZ=1,IZMAX                                           DUM05210
C  CALC SOLID TEMPS                                               DUM05220
      T(N) = WEIGHT*TWALL + (1.0-WEIGHT)*T(N-1)                   DUM05230
      MAX = N-2                                                   DUM05240
      DO 550 I=2,MAX,2                                            DUM05250
      T(I) = 0.5*( T(I+1)+T(I-1) )                                DUM05260
550   CONTINUE                                                    DUM05270
C  NOW, FIND FLOID TEMPS...                                       DUM05280
C  CENTER PLUG DIFFERENT                                          DUM05290
      XI = Q(1)*CP*G                                              DUM05300
      AP = (1.0-EPS(2))*AXS(2)                                    DUM05310
      AP = ISHAPE(ISHAPE)*PI*0.25*APELL*DI*DI*AP                  DUM05320
      DTDZ = HP*AP*( T(2)-T(1) )                                  DUM05330
      DTDZ = DTDZ/XI                                              DUM05340
      T(1) = T(1) + DZ*DTDZ                                       DUM05350
      MAX = N-1                                                   DUM05360
      DO 560 I=3,MAX,2                                            DUM05370
      XI = Q(I)*CP*G                                              DUM05380
      APTOP = ISHAPE(ISHAPE)*(1.0-EPS(I+1))*AXS(I+1)              DUM05390
      APBOT = ISHAPE(ISHAPE)*(1.0-EPS(I-1))*AXS(I-1)              DUM05400
      DTDZ = APTOP*( T(I+1)-T(I) ) - APBOT*( T(I)-T(I-1) )        DUM05410
      DTDZ = DTDZ*HP*0.25*APELL*PI*DI*DI/XI                       DUM05420
      T(I) = T(I) + DZ*DTDZ                                       DUM05430
560   CONTINUE                                                    DUM05440
600   CONTINUE                                                    DUM05450
C  NOW, NEED OUTLET SOLID TEMPS...                                DUM05460
C  SEE NOTE ABOVE RE:  CENTERPOST PLUG                            DUM05470
      T(N) = WEIGHT*TWALL + (1.0-WEIGHT)*T(N-1)                   DUM05480
      MAX = N-2                                                   DUM05490
      DO 610 I=2,MAX,2                                            DUM05500
      T(I) = 0.5*(T(I+1)+T(I-1))                                  DUM05510
610   CONTINUE                                                    DUM05520
C  THAT'S IT!!!                                                   DUM05530
1000  RETURN                                                      DUM05540
      END                                                         DUM05550
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      SUBROUTINE ARR(NA,NB,Q,R,A,R1,R2,RA,RB)                          DDR05560
      DIMENSION RA(100),RB(100)                                        DDR05570
      DIMENSION Q(100),R(100),RR(100),A(100)                           DDR05580
C  CALC  HYDRAULIC RADII, AND ARRAS                                    DDR05590
      N = NA + NB                                                      DDR05600
C  A HALF-CELL                                                         DDR05610
      DO 10 I=2,N,2                                                    DDR05620
      RR(I) = R(I) - RA(I-1)                                           DDR05630
      A(I) = R(I)*R(I) - RA(I-1)*RA(I-1)                               DDR05640
10    CONTINUE                                                         DDR05650
C  B HALF-CELL                                                         DDR05660
      RR(1) = RR(1)                                                    DDR05670
      A(1) = RR(1)*RR(1)                                               DDR05680
      MAX = N-1                                                        DDR05690
      DO 20 I=3,MAX,2                                                  DDR05700
      RR(I) = RR(I) - R(I-1)                                           DDR05710
      A(I) = RR(I)*RR(I) - R(I-1)*R(I-1)                               DDR05720
20    CONTINUE                                                         DDR05730
C  NOW, DETERMIN FLOWS AND POROSITIES OF A AND B SEGS                  DDR05740
C  DEPENDS ON BA AND BB                                                DDR05750
      IF(BA .LE. BB) GOTO 500                                          DDR05760
C  THIS SECTON FOR BA GT BB                                            DDR05770
C  FLOW DISTRIBUTION AND POROSITI                                      DDR05780
      R1 = 0.0                                                         DDR05790
      SUR = 0.0                                                        DDR05800
      DO 100 I=1,N,2                                                   DDR05810
      R1 = R1 + A(I)                                                   DDR05820
100   SUR = SUR + A(I)*RR(I)*RR(I)                                     DDR05830
      DO 110 I=1,N,2                                                   DDR05840
      Q(I) = A(I)*RR(I)*RR(I)/SUR                                      DDR05850
110   CONTINUE                                                         DDR05860
C  B SEGMENT                                                           DDR05870
      R2 = 0.0                                                         DDR05880
      SUR = 0.0                                                        DDR05890
      N1 = N-1                                                         DDR05900
      DO 120 I=2,N1,2                                                  DDR05910
      R2 = R2+A(I)                                                     DDR05920
120   CONTINUE                                                         DDR05930
      XX = A(N-1)* RR(N-1)*RR(N-1)                                     DDR05940
      YY = A(N-3)*RR(N-3)*RR(N-3)                                      DDR05950
      Q(N-1) = Q(N) + Q(N-2)*XX/(XX+YY)                                DDR05960
      XX = A(2)*RR(2)*RR(2)                                            DDR05970
      YY = A(4)*RR(4)*RR(4)                                            DDR05980
      Q(2) = Q(1) + Q(3)*XX/(XX+YY)                                    DDR05990
      MAX = N-3                                                        DDR06000
C  DON'T NEED FOLLOWING IF N .LE. 5                                    DDR06010
      IF(N .LE. 5)GOTO 1000                                            DDR06020
      DO 130 I=4,MAX,2                                                 DDR06030
      YY = A(I)*RR(I)*RR(I)                                            DDR06040
      ZZ = A(I-2)*RR(I-2)*RR(I-2)                                      DDR06050
      Q(I) = Q(I-1) *XX/(XX+YY) + Q(I+1)*YY/(YY+ZZ)                    DDR06060
130   CONTINUE                                                         DDR06070
      GOTO 1000                                                        DDR06080
500   CONTINUE                                                         DDR06090
C  THIS SECTION FOR BA=BB                                              DDR06100
C  FLOW DISTRIBUTION AND POROSITY                                      DDR06110
C  A-SEGMENT                                                           DDR06120
      SUR = 0.0                                                        DDR06130
      R1 = 0.0                                                         DDR06140
      DO 510 I=2,N,2                                                   DDR06150
      R1 = R1 + A(I)                                                   DDR06160
510   SUR = SUR + A(I)*RR(I)*RR(I)                                     DDR06170
      DO 520 I=2,N,2                                                   DDR06180
      Q(I) = A(I)*RR(I)*RR(I)/SUR                                      DDR06190
520   CONTINUE                                                         DDR06200
C  B-SEG                                                               DDR06210
      R2 = 0.0                                                         DDR06220
      SUR = 0.0                                                        DDR06230
      N1 = N-1                                                         DDR06240
      DO 530 I=1,N1,2                                                  DDR06250
      R2 = R2+A(I)                                                     DDR06260
530   CONTINUE                                                         DDR06270
C  TRY SUBDIVIDING BASED ON SQRT(RR)                                   DDR06280
C        --INSTEAD OF A*SQRT(RR)                                       DDR06290
      XX = A(N-1)*RR(N-1)*RR(N-1)                                      DDR06300
      YY = A(N-3)*RR(N-3)*RR(N-3)                                      DDR06310
      Q(N-1) = Q(N) + Q(N-2)*XX/(XX+YY)                                DDR06320
      XX = A(1)*RR(1)*RR(1)                                            DDR06330
      YY = A(3)*RR(3)*RR(3)                                            DDR06340
      Q(1) = Q(2)*XX/(XX+YY)                                           DDR06350
      MAX = N-3                                                        DDR06360
C  DON'T NEED FOLLOWINGIF N .LE. 4                                     DDR06370
      IF( N .LE. 4)GOTO 1000                                           DDR06380
      DO 540 I=3,MAX,2                                                 DDR06390
                                                                       DDR06400
```

```
      XX = A(I)*BB(I)/(A(I)*BB(I)+1.)                                   DUM06410
      TT = A(I-2)*BB(I-2)*BH(I-2)                                       DUM06420
      ZZ = A(I+2)*BH(I+2)*BH(I+2)                                       DUM06430
      Q(I) = Q(I-1)*ZZ/(XX*TT) + Q(I+1)*XX/(ZZ*ZZ)                      DUM06440
540   CONTINUE                                                          DUM06450
1000  RETURN                                                            DUM06460
      END                                                               DUM06470
```

Steady-state Reaction

The procedure here is analogous to the steady-state heat dispersion program. The attached program can simulate either wall-cooled or adiabatic reactors. Details are commented in the listing.

```
C   PROGRAM NAME 'BIMSS2 FORTRAN'                                        BIN00010
C   TREATS 1-ST ORDER INTRINSIC KINETICS                                 BIN00020
C                                                                        BIN00030
C ---------------------------------------------------------------------- BIN00040
C THIS RUN FOR DATA OF TEST CASE                                         BIN00050
C ---------------------------------------------------------------------- BIN00060
C                                                                        BIN00070
C   LAST UPDATE/USE ON 26 JULY 85                                        BIN00080
      DIMENSION Q(100),E(100),A(100),VEL(100)                            BIN00090
      DIMENSION W(100),C(100),T(100)                                     BIN00100
      DIMENSION BA(100),BB(100)                                          BIN00110
      DIMENSION EGLOB(100)                                               BIN00120
      COMMON /BATE/ ZKO,GG                                               BIN00130
      COMMON /BIN/ DELB, DEFF, BHO, CP, BETA                             BIN00140
      COMMON /BX/ BP, BW, TWALL, DT, DP, VPSP                            BIN00150
C   THIS PROGRAM CALCULATES FLOWS AND CONCENTRATIONS GIVEN               BIN00160
C   ARBOLUS DIMENSIONS.                                                  BIN00170
C   VARIABLE **IFLAG**<--IF 0 ==> ADIABATIC REACTOR                      BIN00180
C                       OTHERWISE ==> CONSTANT TWALL                     BIN00190
C   (SEE 'CELLIN' FOR MORE DETAILS)                                      BIN00200
      DATA IFLAG /1/                                                     BIN00210
C----------------------                                                  BIN00220
C-----  USE CGS UNITS-----                                              BIN00230
C-----  TEMP=DEG KELVIN...                                              BIN00240
C-----  CCNC=MOL/CC**3 ...                                              BIN00250
C----------------------                                                  BIN00260
C                                                                        BIN00270
      DATA NLONG,NPRINT /100,5/                                          BIN00280
C   INITIALIZE CONCENTRATION AND TEMPERATURE PROFILES                    BIN00290
      DATA C /100*2.0E-8/                                                BIN00300
      DATA T /100*800.0/                                                 BIN00310
      DATA B /100*0.0/                                                   BIN00320
C   REACTION, HEAT TRANSFER, ETC.,  DATA. . .                          BIN00330
      CIN = C(1)                                                         BIN00340
      TIN = T(1)                                                         BIN00350
      ZKO = 4.5 E8                                                       BIN00360
      GG = 1.2E8                                                         BIN00370
      DELB = 2.5E4                                                       BIN00380
      DEFF = 0.001                                                       BIN00390
      BHO = 9.5 E-8                                                      BIN00400
      CP = 0.25                                                          BIN00410
      BP = .00141                                                        BIN00420
      BW = .2                                                            BIN00430
CCC   BP = 6.32E-4                                                       BIN00440
CCC   BW = 3.17E-4                                                       BIN00450
      TWALL = 400.0                                                      BIN00460
      DT = 3.6                                                           BIN00470
      DP = 0.6                                                           BIN00480
      VPSP = DP/6.0                                                      BIN00490
CCC   QTOT = 81.80                                                       BIN00500
      QTOT = 818.0                                                       BIN00510
      BETA = GELB/ (BHO*CP)                                              BIN00520
      IF(IFLAG .EQ. 0)WRITE(6,3060)                                      BIN00530
      IF(IFLAG .NE. 0)WRITE(6,3070)TWALL                                 BIN00540
C   CALC AREAS BASED ON DTOP AND BA                                      BIN00550
      DTOP = DT / DP                                                     BIN00560
      DO 10 I=1,100                                                      BIN00570
10    W(I) = 20.0                                                        BIN00580
CCC   Z = DTOP + 0.5                                                     BIN00590
C   NOW, TRY ASSIGNING NO. CELLS BASED ON CORRELATION...                 BIN00600
      Z = DTOP/0.816 + 0.5                                               BIN00610
      N = Z                                                              BIN00620
      Z = N                                                              BIN00630
      Z = 0.5*Z                                                          BIN00640
      NB = Z                                                             BIN00650
      NA = N-NB                                                          BIN00660
C   RESTRICT TO EVEN NO. SEGMENTS                                        BIN00670
      IF(NA .GT. NB)NB = NA                                              BIN00680
      N = NA+NB                                                          BIN00690
      WRITE(6,2020)DTOP,N,NA,NB                                          BIN00700
C   SIZE BAGII                                                           BIN00710
C   SET UP TO DO INCREASING EA'S...                                      BIN00720
C   SIZE EVENLY SPACED BAGII                                             BIN00730
      ZN = N/2                                                           BIN00740
      DELB = 1.0/ZN                                                      BIN00750
      B(2) = DELB                                                        BIN00760
      DO 80 I=4,N,2                                                      BIN00770
      B(I) = B(I-2) + DELB                                               BIN00780
80    CONTINUE                                                           BIN00790
C   DETERMINE EPS FOR EACH SEGMENT...                                    BIN00800
```

```
      EBAR = 0.3500                                                     BXN00810
C  VOID FRACTION OF FIRST SEGMENT                                       BXN00820
      CALL VOID(DTDP,0.0,R(2),EBAR,E1)                                  BXN00830
      I=2                                                               BXN00840
      WRITE(6,2010) I,E1                                                BXN00850
100   BA(1) = (1.0-E1)*R(2)*R(2)                                        BXN00860
      BA(1) = SQRT( BA(1) )                                             BXN00870
      BA(2) = R(2)                                                      BXN00880
      BB(1) = E1*R(2)*R(2)                                              BXN00890
      BB(1) = SQRT( BB(1) )                                             BXN00900
      BB(2) = R(2)                                                      BXN00910
      NAX = N-1                                                         BXN00920
      DO 120 I=3,NAX,2                                                  BXN00930
C  VOID FRACTIONS OF RADIAL CELLS BASED ON CORRELATION                  BXN00940
      RHO2 = R(I+1)                                                     BXN00950
      RHO1 = R(I-1)                                                     BXN00960
      CALL VOID(DTDP,RHO1,RHO2,EBAR,EHAT)                               BXN00970
      IW = I+1                                                          BXN00980
      WRITE(6,2010) IW,EBAT                                             BXN00990
      XX = R(I+1)*R(I+1) - R(I-1)*R(I-1)                                BXN01000
      BA(I) = (1.0-EBAT)*XX                                             BXN01010
      BA(I) = BA(I-1)*(I-1) + BA(I)                                     BXN01020
      BA(I) = SQRT( BA(I) )                                             BXN01030
      BA(IW) = R(IW)                                                    BXN01040
      BB(I) = EHAT * XX                                                 BXN01050
      BB(I) = B(I-1)*R(I-1) + BB(I)                                     BXN01060
      BB(I) = SQRT( BB(I) )                                             BXN01070
      BB(IW) = R(IW)                                                    BXN01080
120   CONTINUE                                                          BXN01090
      NAX = N-1                                                         BXN01100
      WRITE(6,2150)                                                     BXN01110
      WRITE(6,2160) (BA(I),R(I+1),I=1,NAX,2)                            BXN01120
      WRITE(6,2160) (BB(I),R(I+1),I=1,NAX,2)                            BXN01130
      CALL ANN(NA,NB,Q,B,A,E1,E2,BA,BB)                                 BXN01140
      B = BA+NB                                                         BXN01150
      DO 200 I=1,N                                                      BXN01160
200   VEL(I) = Q(I)/A(I)                                                BXN01170
C  WRITE RESULTS                                                        BXN01180
      WRITE(6,2050)                                                     BXN01190
      DO 300 I=2,N,2                                                    BXN01200
      J=I-1                                                             BXN01210
      WRITE(6,2060) I,A(I),Q(I),VEL(I),J,A(J),Q(J),VEL(J)               BXN01220
300   CONTINUE                                                          BXN01230
      WRITE(6,2070) E1,E2                                               BXN01240
      WRITE(6,2150)                                                     BXN01250
      WRITE(6,2160) (R(I),I=1,N)                                        BXN01260
      CALL MIXI(NA,NB,Q,2)                                              BXN01270
      WRITE(6,2170)                                                     BXN01280
      WRITE(6,2160) (R(I),I=1,N)                                        BXN01290
      N = NA + NB                                                       BXN01300
C  NOW, CALC CONCENTRATIONS...                                          BXN01310
CCC   WRITE(6,2230)                                                     BXN01320
      WRITE(6,3050)                                                     BXN01330
      KOONT = 0                                                         BXN01340
      NP = 0                                                            BXN01350
500   KOUNT = KOONT+1                                                  BXN01360
      NP = NP + 1                                                       BXN01370
      WRITE(6,2240) KOONT                                               BXN01380
      IF(KCONT .GT. NLONG)GOTO 1000                                     BXN01390
C  A-HALF-CELL                                                          BXN01400
      CALL CELLIN(1,N,QTOT,Q,T,C,IFLAG,RA,RB,RGLOB,OZLZ)                BXN01410
      IF(NP .LT. NPRINT)GOTO 550                                        BXN01420
      WRITE(6,3000)                                                     BXN01430
      WRITE(6,3030)                                                     BXN01440
      CABAR = 0.0                                                       BXN01450
      TABAR = 0.0                                                       BXN01460
      RTOT = 0.0                                                        BXN01470
      DO 520 I=2,N,2                                                    BXN01480
      CABAR = CABAR + C(I)*Q(I)                                         BXN01490
      TABAR = TABAR + T(I)*Q(I)                                         BXN01500
      II = I-1                                                          BXN01510
      WRITE(6,2255) II,T(II)                                            BXN01520
      RWBITS = RGLOB(I)*OZLZ                                            BXN01530
      RTOT = RTOT + RWBITS                                              BXN01540
      WRITE(6,2250) I,C(I),T(I),RWBITS                                  BXN01550
520   CONTINUE                                                          BXN01560
      WRITE(6,3040) CABAR,TABAR,RTOT                                    BXN01570
C                                                                       BXN01580
      CONV = 1.0 - CABAR/CIN                                            BXN01590
      WRITE(6,3045) CONV                                                BXN01600
```

```
      GO TO 700
C   NOW, SIZING AT B-INLET                                              BIN01610
      CALL SIZ2(0,NA,NB,Q,W,C)                                          BIN01620
      CALL SIZ2(0,NA,NB,Q,W,T)                                          BIN01630
CCC   WRITE(6,3010)                                                     BIN01640
CCC   WRITE(6,3020)                                                     BIN01650
700   CONTINUE                                                          BIN01660
C   NOW B-HALF-CELL                                                     BIN01670
      CALL CELLIN(0,W,QTOT,Q,T,C,IFLAG,BA,BB,BGLCB,DELZ)                BIN01680
      IF(BB .LT. NPBINT)GOTO 750                                        BIN01690
      WRITE(6,3010)                                                     BIN01700
      WRITE(6,3030)                                                     BIN01710
      CBBAR = 0.0                                                       BIN01720
      TBBAR = 0.0                                                       BIN01730
      BTOT = 0.0                                                        BIN01740
      DO 720 I=1,NB,2                                                   BIN01750
      I1 = I+1                                                          BIN01760
      CBBAR = CBBAR + C(I)*Q(I)                                         BIN01770
      TBBAR = TBBAR + T(I)*Q(I)                                         BIN01780
      BWBITE = DELZ * BGLOB(I)                                          BIN01790
      BTOT = BTOT + BWBITE                                              BIN01800
      WRITE(6,2250)I,C(I),T(I),BWBITE                                   BIN01810
      WRITE(6,2255)I1,T(I1)                                             BIN01820
720   CONTINUE                                                          BIN01830
      WRITE(6,3040)CBBAR,TBBAR,BTOT                                     BIN01840
      CONV = 1.0 - CBBAR/CIN                                            BIN01850
      WRITE(6,3045)CONV                                                 BIN01860
      NB = 0                                                            BIN01870
750   CONTINUE                                                          BIN01880
C   NOW, SIZING AT A-INLET                                              BIN01890
      CALL SIZ2(1,BA,NB,Q,W,C)                                          BIN01900
      CALL SIZ2(1,NA,NB,Q,W,T)                                          BIN01910
      GOTO 500                                                          BIN01920
1000  CONTINUE                                                          BIN01930
C   FORMATS. . .                                                        BIN01940
2010  FORMAT(' I =',I6,'  EPS = ',E11.4)                                BIN01950
2015  FORMAT(' ALPHA =',E11.4)                                          BIN01960
2020  FORMAT(' DTDP = ',E11.4,'  N =',I3,' NA =',I3,' NB =',I3)         BIN01970
2030  FORMAT(' D1/R =',E11.4)                                           BIN01980
2040  FORMAT(' F = ',E11.4)                                             BIN01990
2050  FORMAT(20I,'A',63X,'B',/,2X,40('-'),2I,40('-'),/,                 BIN02000
     1 2(2I,'I',7I,'A',11I,'F',9I,'FEL  ',5I),/,                        BIN02010
     2 1I,2('----',2X,3('----------',2X)))                              BIN02020
2060  FORMAT(1X,2(I3,2X,3(E10.4,2X)))                                   BIN02030
2070  FORMAT(' S1 = ',E11.4,'  S2 = ',E11.4)                            BIN02040
2150  FORMAT(' BADII...')                                               BIN02050
2160  FORMAT(5(2I,E11.4))                                               BIN02060
2170  FORMAT(' SIZING WEIGHT FACTORS. . .')                             BIN02070
2230  FORMAT(9I,'A',30I,'B',/,2(2I,29('-')),/,                          BIN02080
     1 2I,2(1I,'I',8I,'C',7I,3I,'C/CATG',4I),/,                         BIN02090
     2 2I,2('---',2X,'----------',2I,'----------',2X))                  BIN02100
C23456789.123456789.123456789.123456789.123456789.123456789.          BIN02110
2240  FORMAT(' CELL NO ',I5)                                            BIN02120
2250  FORMAT(I5,3(2X,E13.6))                                            BIN02130
2255  FORMAT(I5,15X,E13.6)                                              BIN02140
2260  FORMAT(' NA = ',E11.4,'  BBEC = ',E11.4)                          BIN02150
2270  FORMAT(' CALC. INVALID VOID FRACT.  PGM ABORTED ')                BIN02160
2290  FORMAT(' F =',E11.4,' SOM =',E11.4,' EPS1 =',E11.4)               BIN02170
3000  FORMAT(' A-HALF-CELL ')                                           BIN02180
3010  FORMAT(' B-HALF-CELL ')                                           BIN02190
3020  FORMAT(' -----INLET')                                             BIN02200
3030  FORMAT(' -----OUTLET')                                            BIN02210
3040  FORMAT(' CBOLK =',E13.6,' TBOLK=',E13.6,' RTOT=',E13.6)           BIN02220
3045  FORMAT(' CONVERSION = ',E13.6)                                    BIN02230
3050  FORMAT(' I...C...T...BATE(MOLE/SEC)... ')                         BIN02240
3060  FORMAT(5(' *'),' ADIABATIC REACTOR',5(' *'))                      BIN02250
3070  FORMAT(5(' *'),' WALL-COOLED...TWALL(DEG-R) = ',E13.6)            BIN02260
      STOP                                                              BIN02270
      END                                                               BIN02280
C                                                                       BIN02290
      SUBROUTINE ANN(NA,NB,Q,R,A,E1,E2,BA,BB)                           BIN02300
      DIMENSION BA(100),BB(100)                                         BIN02310
      DIMENSION Q(100),R(100),BN(100),A(100)                            BIN02320
C   CALC  HYDRAULIC BADII, AND AREAS                                    BIN02330
      N = NA + NB                                                       BIN02340
C   A HALF-CELL                                                         BIN02350
      DO 10 I=2,N,2                                                     BIN02360
      BN(I) = R(I) - BA(I-1)                                            BIN02370
      A(I) = R(I)*BN(I) - BA(I-1)*BA(I-1)                               BIN02380
10    CONTINUE                                                          BIN02390
                                                                        BIN02400
```

```
C  B HALF-CELL                                                        BXN02410
       BH(1) = BB(1)                                                 BXN02420
       A(1) = BB(1)*BB(1)                                            BXN02430
       MAX = N-1                                                     BXN02440
       DO 20 I=3,MAX,2                                               BXN02450
       BH(I) = BH(I-2) - B(I-1)                                      BXN02460
       A(I) = BB(I)*BB(I) - B(I-1)*B(I-1)                            BXN02470
20     CONTINUE                                                      BXN02480
C  NOW, DETERMINE FLOWS AND POROSITIES OF A AND B SEGS               BXN02490
C  DEPENDS ON NA AND NB                                              BXN02500
       IF(NA .LE. NB) GOTO 500                                       BXN02510
C  THIS SECTION FOR NA GT NB                                         BXN02520
C  FLOW DISTRIBUTION AND POROSITY                                    BXN02530
       Z1 = 0.0                                                      BXN02540
       SUM = 0.0                                                     BXN02550
       DO 100 I=1,N,2                                                BXN02560
       Z1 = Z1 + A(I)                                                BXN02570
100    SUM = SUM + A(I)*SQRT(BH(I))                                  BXN02580
       DO 110 I=1,N,2                                                BXN02590
       Q(I) = A(I)*SQRT(BH(I))/SUM                                   BXN02600
110    CONTINUE                                                      BXN02610
C  B SEGMENT                                                         BXN02620
       Z2 = 0.0                                                      BXN02630
       SUM = 0.0                                                     BXN02640
       N1 = N-1                                                      BXN02650
       DO 120 I=2,N1,2                                               BXN02660
       Z2 = Z2+A(I)                                                  BXN02670
120    CONTINUE                                                      BXN02680
       XX = A(N-1)*SQRT( BH(N-1) )                                   BXN02690
       YY = A(N-3)*SQRT( BH(N-3) )                                   BXN02700
       Q(N-1) = Q(N) + Q(N-2)*XX/(XX+YY)                             BXN02710
       XX = A(2)*SQRT(BH(2))                                         BXN02720
       YY = A(4)*SQRT(BH(4))                                         BXN02730
       Q(2) = Q(1) + Q(3)*XX/(XX+YY)                                 BXN02740
       MAX = N-3                                                     BXN02750
C  DON'T NEED FOLLOWING IF N .LE. 5                                  BXN02760
       IF(N .LE. 5) GOTO 1000                                        BXN02770
       DO 130 I=4,MAX,2                                              BXN02780
       XX = A(I)*SQRT(BH(I))                                         BXN02790
       YY = A(I-2)*SQRT(BH(I-2))                                     BXN02800
       ZZ = A(I+2)*SQRT(BH(I+2))                                     BXN02810
       Q(I) = Q(I-1)*XX/(XX+YY) + Q(I+1)*YY/(YY+ZZ)                  BXN02820
130    CONTINUE                                                      BXN02830
       GOTO 1000                                                     BXN02840
500    CONTINUE                                                      BXN02850
C  THIS SECTION FOR NA=NB                                            BXN02860
C  FLOW DISTRIBUTION AND POROSITY                                    BXN02870
C  A-SEGMENT                                                         BXN02880
       SUM = 0.0                                                     BXN02890
       Z1 = 0.0                                                      BXN02900
       DO 510 I=2,N,2                                                BXN02910
       Z1 = Z1 + A(I)                                                BXN02920
510    SUM = SUM + A(I)*SQRT(BH(I))                                  BXN02930
       DO 520 I=2,N,2                                                BXN02940
       Q(I) = A(I)*SQRT(BH(I))/SUM                                   BXN02950
520    CONTINUE                                                      BXN02960
C  B-SEG                                                             BXN02970
       Z2 = 0.0                                                      BXN02980
       SUM = 0.0                                                     BXN02990
       N1 = N-1                                                      BXN03000
       DO 530 I=1,N1,2                                               BXN03010
       Z2 = Z2+A(I)                                                  BXN03020
530    CONTINUE                                                      BXN03030
C  TRY SOMETHING BASED ON SQRT(BH)                                   BXN03040
C        --INSTEAD OF A*SQRT(BH)                                     BXN03050
       XX = A(N-1)*SQRT(BH(N-1))                                     BXN03060
       YY = A(N-3)*SQRT(BH(N-3))                                     BXN03070
       Q(N-1) = Q(N) + Q(N-2)*XX/(XX+YY)                             BXN03080
       XX = A(1)*SQRT(BH(1))                                         BXN03090
       YY = A(3)*SQRT(BH(3))                                         BXN03100
       Q(1) = Q(2)*XX/(XX+YY)                                        BXN03110
       MAX = N-3                                                     BXN03120
C  DON'T NEED FOLLOWINGIF N .LE. 4                                   BXN03130
       IF( N .LE. 4)GOTO 1000                                        BXN03140
       DO 540 I=3,MAX,2                                              BXN03150
       XX = A(I)*SQRT(BH(I))                                         BXN03160
       YY = A(I-2)*SQRT(BH(I-2))                                     BXN03170
       ZZ = A(I+2)*SQRT(BH(I+2))                                     BXN03180
       Q(I) = Q(I-1)*XX/(XX+YY) + Q(I+1)*XX/(XX+ZZ)                  BXN03190
540    CONTINUE                                                      BXN03200
```

```
 1000   RETURN                                                          BIN03210
        END                                                             BIN03220
 C                                                                      BIN03230
        SUBROUTINE VOID(DTDP,RBO1,RBO2,EBAB,EPS)                        BIN03240
        PI = 2.0*ARSIN(1.0)                                             BIN03250
        A1 = 0.3463                                                     BIN03260
        A2 = 0.4271                                                     BIN03270
        A3 = 2.4509                                                     BIN03280
        A4 = 2.2011                                                     BIN03290
        ALP = 0.5*DTDP* A2                                              BIN03300
        B = (A3 - A4) *PI*DTDP/2.0                                      BIN03310
        C = A3 * PI * DTDP / 2.0                                        BIN03320
        A = A1 * (1.0-EBAB) * EXP(-1.0*ALP)                             BIN03330
 CCC    WRITE(6,2000)A,ALP,B,C,DTDP                                     BIN03340
        R2 = RBO2                                                       BIN03350
        R1 = RBO1                                                       BIN03360
        VADD = 0.0                                                      BIN03370
        Y = 0.0                                                         BIN03380
        TEST = 1.0-0.5/DTDP                                             BIN03390
        IF(RBO2 .LE. TEST)GOTO 100                                      BIN03400
 C  THIS SECTION TREATS OUTTERMOST ANNULUS.  VOID BETWEEN               BIN03410
 C      WALL AND 0.25DP HAS DIFFERENT FUNCTION....                      BIN03420
        VADD = 0.5 - 0.29479*(1.0-EBAB)                                 BIN03430
        VADD = VADD*DTDP - 0.125                                        BIN03440
        VADD = VADD/(DTDP*DTDP)                                         BIN03450
        R2 = TEST                                                       BIN03460
        IF(RBO1 .GE. TEST)GOTO 200                                      BIN03470
 100    CONTINUE                                                        BIN03480
        Y = 0.5*EBAB*(R2*R2-R1*R1)                                      BIN03490
        ARG = B-C*R2                                                    BIN03500
        F2 = ALP*COS(ARG) - C*SIN(ARG)                                  BIN03510
        F2 = F2 * EXP( ALP*R2 )                                         BIN03520
        ARG = B-C*R1                                                    BIN03530
        F1 = ALP*CCS(ARG) - C*SIN(ARG)                                  BIN03540
        F1 = F1*EXP( ALP*R1 )                                           BIN03550
        Y = Y + (F2-F1)*A/(ALP*ALP + C*C)                               BIN03560
 200    VVOID = 2.0*(Y + VADD)                                          BIN03570
        VTOT = RBO2*RBO2 - RBO1*RBO1                                    BIN03580
        EPS = VVOID/VTOT                                                BIN03590
 C2000  FORMAT(' A, ALP, B, C, DTDP = . .',/,5(2X,E11.4) )              BIN03600
        RETURN                                                          BIN03610
        END                                                             BIN03620
 C                                                                      BIN03630
 C                                                                      BIN03640
        SUBROUTINE MIX1(NA,NB,Q, W)                                     BIN03650
 C  THIS SUBROUTINE DETERMINES WEIGHT FACTORS FOR                       BIN03660
 C  MIXING AT ANNULUS INLETS                                            BIN03670
        DIMENSION Q(100),W(100)                                         BIN03680
        N = NA+NB                                                       BIN03690
        IF(NA .LE. NB) GOTO 200                                         BIN03700
 C  THIS SECTION FOR NA GT NB                                          BIN03710
 C  NEED WEIGHTS FOR ODD NUMBERED SEGMENTS                              BIN03720
        W(N) = 0.0                                                      BIN03730
        W(1) = 1.0                                                      BIN03740
        N2 = N-2                                                        BIN03750
        DO 10 I=3,N2,2                                                  BIN03760
        I1 = N2 - I + 3                                                 BIN03770
        W(I1) = ( Q(I1+1) - (1.0-W(I1+2))*Q(I1+2) )/Q(I1)               BIN03780
 10     CONTINUE                                                        BIN03790
        GOTO 1000                                                       BIN03800
 200    CONTINUE                                                        BIN03810
 C  THIS SECTION FOR NA = NB                                           BIN03820
 C  NEED WEIGHTS FOR EVEN NUMBERED SEGMENTS                             BIN03830
        W(N) = 0.0                                                      BIN03840
        N2 = N-2                                                        BIN03850
        DO 300 I=2,N2,2                                                 BIN03860
        I1 = 2-I+N2                                                     BIN03870
        W(I1) = ( Q(I1+1) - (1.0-W(I1+2))*Q(I1+2) )/Q(I1)               BIN03880
 300    CONTINUE                                                        BIN03890
 1000   CONTINUE                                                        BIN03900
        RETURN                                                          BIN03910
        END                                                             BIN03920
        SUBROUTINE MIX2(ITRANS,NA,NB,Q,R,C)                             BIN03930
        DIMENSION W(100),Q(100),C(100)                                  BIN03940
 C  THIS SUBROUTINE DETERMINES ANNULUS INLET CONCENTRATIONS             BIN03950
 C  ITRANS=0==>A TO B TRANSITION                                        BIN03960
 C      =1==>B TO A TRANSITION                                          BIN03970
        N = NA+NB                                                       BIN03980
        IF(NA .LE. NB)GOTO 500                                          BIN03990
 C  THIS SECTION FOR NA GT NB                                           BIN04000
```

```
      IF(ITRANS .NE. 0)GOTO 200                                          BIN04010
C  A TO B TRANS                                                          BIN04020
C  B'S ARE EVEN NUMBERED SOBSCRIPTS                                       BIN04030
      N1 = N-1                                                           BIN04040
      DO 100 I=2,N1,2                                                    BIN04050
      C(I) = (1.0-W(I+1))*Q(I+1)*C(I+1)                                  BIN04060
      C(I) = C(I) + W(I-1)*Q(I-1)*C(I-1)                                 BIN04070
      C(I) = C(I) / Q(I)                                                 BIN04080
100   CONTINUE                                                           BIN04090
      RETURN                                                             BIN04100
200   CONTINUE                                                           BIN04110
C  B TO A TRANS                                                          BIN04120
C  A'S ARE ODD NUMBERED SUBSCRIPTS                                        BIN04130
      C(1) = C(2)                                                        BIN04140
      C(N) = C(N-1)                                                      BIN04150
      N2 = N-2                                                           BIN04160
      DO 300 I=3,N2,2                                                    BIN04170
      C(I) = (1.0-W(I))*C(I-1) + W(I)*C(I+1)                             BIN04180
300   CONTINUE                                                           BIN04190
      RETURN                                                             BIN04200
500   CONTINUE                                                           BIN04210
C  THIS SECTION FOR BA=BB                                                BIN04220
      IF(ITRANS .NE. 0)GOTO 700                                          BIN04230
C  A TO B TRANS                                                          BIN04240
C  B'S ARE ODD NUMBERED SUBSCRIPTS                                        BIN04250
      C(1) = C(2)                                                        BIN04260
      N1 = N-1                                                           BIN04270
      DO 600 I=3,N1,2                                                    BIN04280
      C(I) = (1.0-W(I+1))*Q(I+1)*C(I+1)                                  BIN04290
      C(I) = C(I) + W(I-1)*Q(I-1)*C(I-1)                                 BIN04300
      C(I) = C(I) / Q(I)                                                 BIN04310
600   CONTINUE                                                           BIN04320
      RETURN                                                             BIN04330
700   CONTINUE                                                           BIN04340
C  B TO A TRANSITION                                                     BIN04350
C  A'S EVEN NUMBERED SUBSCRIPTS                                           BIN04360
      C(N) = C(N-1)                                                      BIN04370
      N2 = N-2                                                           BIN04380
      DO 800 I=2,N2,2                                                    BIN04390
      C(I) = W(I)*C(I+1) + (1.0-W(I))*C(I-1)                             BIN04400
800   CONTINUE                                                           BIN04410
      RETURN                                                             BIN04420
      END                                                                BIN04430
      FONCTION TCAT(C,T)                                                 BIN04440
      COMMCN /BATE/ ZKO,GG                                               BIN04450
      COMMCN /BZM/ OELH, DEFF, BHO, CP, BETA                             BIN04460
      COMMCN /HX/ HP, HW, TWALL, DT, DP, VPSP                            BIN04470
      XI = GG / (2.0*T*T)                                                BIN04480
      BJUNK = HP/(DELH*SQRT(DEFF))                                       BIN04490
      YY = BJUNK/( C * SQRT( XK(T) ) )                                   BIN04500
      DELT = 1.0/(YY - XI)                                               BIN04510
      IF(DELT .GT. 0)GOTO 200                                            BIN04520
C IN HERE, OUT OF RANGE OF LINEARIZATION...OR ELSE, STABILITY PROBS      BIN04530
      WRITE(6,100)                                                       BIN04540
100   FORMAT(' ---PGM ABORT IN FONC -TCAT- ---'*//,                      BIN04550
     1 ' ---BEYOND LINEARIZ. RANGE ---'//,                               BIN04560
     2 ' ---OR, STABILITY PROBLEMS ---')                                 BIN04570
      STOP                                                               BIN04580
200   CONTINUE                                                           BIN04590
      TCAT = T + DELT                                                    BIN04600
      RETURN                                                             BIN04610
      END                                                                BIN04620
C                                                                        BIN04630
      FONCTION XK(T)                                                     BIN04640
      COMMCN /BATE/ ZKO, GG                                              BIN04650
      XK = ZKO / EXP(GG/T)                                               BIN04660
      RETURN                                                             BIN04670
      END                                                                BIN04680
C                                                                        BIN04690
      SOBROUTINE CELLIN(ITRANS,N,QTOT,Q,T,C,IFLAG,BA,BB,BGLOB,DELZ)      BIN04700
C  VARIABLE **IFLAG** -- IF 0 ==> ADIABATIC REACTOR                      BIN04710
C                        OTHERWISE ==> CONSTANT TWALL                    BIN04720
      COMMCN /BZM/ DELH, DEFF, BHO, CP, BETA                             BIN04730
      COMMCN /BATE/ ZKO, GG                                              BIN04740
      COMMCN /HX/ HP, HW, TWALL, DT, OP, VPSP                            BIN04750
      DIMENSION T(100),C(100),Q(100)                                     BIN04760
      DIMENSION BA(100),BB(100)                                          BIN04770
      DIMENSION BGLOB(100)                                               BIN04780
C                                                                        BIN04790
C  SET OP NUMERICAL INTEGRATION PARAMETERS                               BIN04800
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```
      PI = 3.1416                                                       BIN04810
      NDIV = 1                                                          BIN04820
      IX = NDIV                                                         BIN04830
      DELZ = 0.816 * DP /IX                                             BIN04840
C  ITBANS     =0==>B HALF-CELL                                         BIN04850
C            .NE. 0==>A HALF-CELL                                      BIN04860
      IF(ITBANS .NE. 0)GOTO 1000                                        BIN04870
C  B HALF-CELL                                                         BIN04880
CCC   WRITE(6,101)                                                      BIN04890
C101   FORMAT(' ...IN B-CALCNS...')                                    BIN04900
      NAXIZ = NDIV                                                      BIN04910
      DO 500 IZ = 1,NAXIZ                                               BIN04920
C  CALC PELLET TEMPS                                                   BIN04930
CCC   WRITE(6,2000) (I,T(I),C(I),I=1,N)                                BIN04940
      CALL TPELL(ITBANS,N,QTOT,Q,T,C,IFLAG,BA,BB, 2000.0, 2000.0)       BIN04950
CCC   WRITE(6,2000) (I,T(I),C(I),I=1,N)                                BIN04960
C  CALC CCSC DEBIVS AND NEW C'S AND T'S                                BIN04970
      AREA = 0.5 * BB(1)*BB(1)*PI*0.25*DT*DT/VPSP                       BIN04980
      CSTOFF = AREA * SQRT(DEFF)                                        BIN04990
      BGLOB(1) = CSTOFF*C(1)*SQRT( XK(T(2)) )                           BIN05000
      DELC = DELZ*(-1.0*BGLOB(1))/( QTOT*Q(1) )                         BIN05010
      C(1) = C(1) + DELC                                                BIN05020
      XIZ = RHO*CP*Q(1)*QTOT                                            BIN05030
      DELT = DELZ * AREA * HP * ( T(2) - T(1) )/XIZ                     BIN05040
      T(1) = T(1) + DELT                                                BIN05050
      NAX = N-1                                                         BIN05060
      DO 200 I=3,NAX,2                                                  BIN05070
      ABOT = BB(I-1)*BB(I-1) - BB(I-2)*BB(I-2)                          BIN05080
      ABOT = 0.5 * ABOT * PI * 0.25 * DT * DT / VPSP                    BIN05090
      ATOP =BB(I+1)*BB(I+1) - BB(I)*BB(I)                               BIN05100
      ATOP =0.5 * ATOP * PI * 0.25 * DT * DT / VESP                     BIN05110
      II = ABOT * SQRT( XK(T(I-1)) )                                    BIN05120
      IX = ATOP * SQRT( XK(T(I+1)) ) + II                               BIN05130
      BGLOB(I) =  IX * C(I) * SQRT(DEFF)                                BIN05140
      DELC = DELZ * (-1.0*BGLOB(I)) / (QTOT*Q(I))                       BIN05150
      C(I) = C(I) + DELC                                                BIN05160
      DTDZ = ATOP*(T(I+1)-T(I)) + ABOT*(T(I-1)-T(I))                    BIN05170
      XIZ = RHO*CP*Q(I)*QTOT                                            BIN05180
      DELT = DELZ * DTDZ * HP /XIZ                                      BIN05190
      T(I) = T(I) + DELT                                                BIN05200
200   CONTINUE                                                          BIN05210
C  NOW, NEED PELLET TEMPS AT OUTLET                                    BIN05220
CCC   WRITE(6,2000) (I,T(I),C(I),I=1,N)                                BIN05230
      CALL TPELL(ITBANS,N,QTOT,Q,T,C,IFLAG,BA,BB,2000.0, 2000.0)        BIN05240
CCC   WRITE(6,2000) (I,T(I),C(I),I=1,N)                                BIN05250
CCC   DO 400 I=1,N                                                      BIN05260
CCC   WRITE(6,2000)I,T(I),C(I)                                          BIN05270
C400   CONTINUE                                                        BIN05280
500   CONTINUE                                                          BIN05290
      RETURN                                                            BIN05300
C                                                                       BIN05310
1000  CONTINUE                                                          BIN05320
C  THIS SECTION FOR A HALF-CELL                                        BIN05330
CCC   WRITE(6,1001)                                                     BIN05340
C1001   FORMAT(' ...IN A-CLACNS...')                                   BIN05350
      DO 1500 IZ = 1,NDIV                                               BIN05360
      TN1OLD = T(N-1)                                                   BIN05370
      CNOLD = C(N)                                                      BIN05380
C  GET PELLET TEMPS                                                    BIN05390
CCC   WRITE(6,2000) (I,T(I),C(I),I=1,N)                                BIN05400
      CALL TPELL(ITBANS,N,QTOT,Q,T,C,IFLAG,BA,BB,TN1OLD,CN1OLD)        BIN05410
CCC   WRITE(6,2000) (I,T(I),C(I),I=1,N)                                BIN05420
C  CALC CONC'N DEBIVS AND C'S AND T'S                                  BIN05430
      NAX = N-2                                                         BIN05440
      DO 1200 I=2,NAX,2                                                 BIN05450
      IF(I .GT. 2)GOTO 1140                                             BIN05460
      ABOT = 0.5 * BA(1)*BA(1) * PI * 0.25 * DT * DT /VPSP              BIN05470
      GOTO 1150                                                         BIN05480
1140  CONTINUE                                                          BIN05490
      ABOT = BA(I-1)*BA(I-1) - BA(I-2)*BA(I-2)                          BIN05500
      ABOT = 0.5 * ABOT * PI * 0.25 * DT * DT /VPSP                     BIN05510
1150  CONTINUE                                                          BIN05520
      ATOP = BA(I+1)*BA(I+1) - BA(I)*BA(I)                              BIN05530
      ATOP = 0.5 * ATOP * PI * 0.25 * DT * DT / VPSP                    BIN05540
      II = ABOT * SQRT( XK(T(I-1)) )                                    BIN05550
      IX = ATOP * SQRT( XK(T(I+1)) ) + II                               BIN05560
      BGLOB(I) = IX * C(I) * SQRT(DEFF)                                 BIN05570
      DELC = DELZ* (-1.0*BGLOB(I)) / (QTOT*Q(I))                        BIN05580
      C(I) = C(I) + DELC                                                BIN05590
      DTDZ = ATOP*(T(I+1)-T(I)) + ABOT*(T(I-1)-T(I))                    BIN05600
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      XIZ = RHO*CP*Q(I)*QTOT                                            BIX05610
      DELT =  BP * DELZ * DTDZ/XIZ                                      BIX05620
      T(I) = T(I) + DELT                                                BIX05630
 1200 CONTINUE                                                          BIX05640
C                                                                       BIX05650
C  OUTERMOST PLOG EFFECTED BY WALL ALSO                                 BIX05660
      XX = SQRT(DEFF * XK(T(N-1)) )                                     BIX05670
      XIZ = BA(N-1)*BA(N-1) - BA(N-2)*BA(N-2)                           BIX05680
      AREA = 0.5 * PI * 0.25 * DT * DT * XIZ / VPSP                     BIX05690
      BGLOS(N) =  XI * AREA * C(N)                                      BIX05700
      DELC = DELZ * (-1.0*BGLOS(N)) / (QTOT*Q(N))                       BIX05710
      C(N) = C(N) + DELC                                                BIX05720
      IF(IFLAG .EQ. 0)GOTO 1300                                         BIX05730
      XIZ = RHO * CP * Q(N) * QTOT                                      BIX05740
      ALF = PI * BP * DT / XIZ                                          BIX05750
      XI = XK( TS10LD )                                                 BIX05760
      XI = DELH * SQRT(DEFF*XI) * CHOLD / XIZ                           BIX05770
      XI = XI*PI*0.25*DT*DT *(BA(N-1)*BA(N-1)-BA(N-2)*BA(N-2)) /VPSP    BIX05780
      XI = XI / 2.0                                                     BIX05790
      DTDZ = XI - ALF * ( T(N)-TWALL )                                  BIX05800
      T(N) = T(N) + DELZ * DTDZ                                         BIX05810
      IF(T(N) .LT. TWALL)T(N) = TWALL                                   BIX05820
      GOTO 1310                                                         BIX05830
C  THIS SECTION FOR ADIABATIC REACTOR                                   BIX05840
 1300 CONTINUE                                                          BIX05850
      AREA = 0.5*PI*0.25*DT*DT *(BA(N-1)*BA(N-1)-BA(N-2)*BA(N-2))/VPSP  BIX05860
      XIZ = RHO*CP*Q(N)*QTOT                                            BIX05870
      DELT = AREA*BP*DELZ*(T(N-1)-T(N))/XIZ                             BIX05880
      T(N) = T(N) + DELT                                                BIX05885
 1310 CONTINUE                                                          BIX05890
CCC   DO 1400 I=1,N                                                     BIX05900
CCC   WRITE(6,2000)I,T(I),C(I)                                          BIX05910
C1400 CONTINUE                                                          BIX05920
C  NOW, NEED PELLET TEMPS AT OUTLET                                     BIX05930
CCC   WRITE(6,2000) (I,T(I),C(I),I=1,N)                                 BIX05940
      CALL TPELL(ITRANS,N,QTOT,Q,T,C,IFLAG,BA,BB,TS10LD,CN10LD)         BIX05950
CCC   WRITE(6,2000) (I,T(I),C(I),I=1,N)                                 BIX05960
 1500 CONTINUE                                                          BIX05970
 2000 FORMAT(/,(I5,2X,E13.6,2X,E13.6))                                  BIX05980
      RETURN                                                            BIX05990
      END                                                               BIX06000
      SUBROUTINE TPELL(ITRANS,N,QTOT,Q,T,C,IFLAG,BA,BB,TS10LD,CN10LD)   BIX06010
      DIMENSION Q(100),T(100),C(100),BA(100),BB(100)                    BIX06020
      COMMON /BXS/ DELH, DEFF, RHO, CP, BETA                            BIX06030
      COMMON /BAZZ/ XKO, GG                                             BIX06040
      COMMON /HX/ HP, HW, TWALL, DT, DP, VPSP                           BIX06050
C  VARIABLE ITRANS--IF 0 ==>B-HALF-CELL                                 BIX06060
C                    OTHERWISE ==>A-HALF-CELL                         BIX06070
      IF(ITRANS .NE. 0)GOTO 100                                         BIX06080
C  THIS SECTION FOR B-HALF-CELL                                         BIX06090
C  CALC PELLET TEMPS                                                    BIX06100
      NAX = N-2                                                         BIX06110
      DO 100 I=2,NAX,2                                                  BIX06120
      TSTAB = 0.5*( T(I+1)+T(I-1) )                                     BIX06130
      CSTAB = 0.5*( C(I+1)+C(I-1) )                                     BIX06140
      T(I) = TCAT(CSTAB,TSTAB)                                          BIX06150
 100  CONTINUE                                                          BIX06160
C  CALC WALL SOLID PLUG TEMP--FOR CF WALL TEMP, TOO.                    BIX06170
      IF (IFLAG .EQ. 0 )GOTO 140                                        BIX06180
      XI = XK( T(N-1) )                                                 BIX06190
      XI = SQRT(DEFF*XI)                                                BIX06200
      XI = DELH * XI * C(N-1) / HP                                      BIX06210
      YY = 0.5 * GG /( T(N-1)*T(N-1) )                                  BIX06220
      BOT = XI * YY - 1.1                                               BIX06230
      TOP = T(N-1)*( XI*YY - 1.0 )                                      BIX06240
      TOP = TOP - 0.1*TWALL - XI                                        BIX06250
      T(N) = TOP / BOT                                                  BIX06260
      GOTO 150                                                          BIX06270
 140  CONTINUE                                                          BIX06280
      T(N) = TCAT( C(N-1), T(N-1) )                                     BIX06290
 150  CONTINUE                                                          BIX06300
      RETURN                                                            BIX06310
C  THIS SECTION FOR A-HALF-CELL                                         BIX06320
 900  CONTINUE                                                          BIX06330
      T(1) = TCAT( C(2), T(2) )                                         BIX06340
      NAX = N-1                                                         BIX06350
      DO 1100 I=3,NAX,2                                                 BIX06360
      CSTAB = 0.5*( C(I-1)+C(I+1) )                                     BIX06370
      TSTAB = 0.5*( T(I-1)+T(I+1) )                                     BIX06380
      T(I) = TCAT( CSTAB,TSTAB )                                        BIX06390
                                                                        BIX06400
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 1100  CONTINUE                                                        BXN06410
       RETURN                                                          BXN06420
       END                                                             BXN06430
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Steady-state Reaction (Fickian)

The implicit method (Lee, 1985; Hornbeck, 1975) yields tri-diagonal matrices (of dimension equal to the number of radial increments plus one) which must be inverted at each axial position to yield concentration and temperature vectors. The matrices are simple to invert because of their band characteristic (Hornbeck, 1975). The attached program simulates either adiabatic (hw=0) or wall-cooled (hw=value) reactors. Comments within the listing explain other program steps.

```
C  PROGRAM NAME 'FICK2D FORTRAN'                                                  FIC00010
C  USES FICKIAN ANALOGY WITH RADIAL DISPERSION ONLY                               FIC00020
C  TO GET CONCENTRATION AND TEMPERATURE PROFILES IN PACKED BED REACTOR            FIC00030
C                                                                                 FIC00040
      IMPLICIT REAL*8 (A-H,O-Z)                                                   FIC00050
      DIMENSION A(21), B(21), C(21), E(21), CCALL(21), ACALL(21)                  FIC00060
      DIMENSION COLO(21), CNEW(21), TOLO(21), TNEW(21), TCALL(21)                 FIC00070
      COMMON /BIG/ OSCAT, VPSP, DELH, HF, EKO, GG, CIN                            FIC00080
      WRITE(6,2000)                                                               FIC00090
C                                                                                 FIC00100
C  TEST CASE                                                                      FIC00110
C                                                                                 FIC00120
C  VARIABLE LIMIT...IF 0==>NO DIFF'N LIMITATION                                   FIC00130
C                   OTHERWISE==>IS DIFF'N LIMITATION                              FIC00140
      LIMIT = 1                                                                   FIC00150
C                                                                                 FIC00160
C  INPUT DATA                                                                     FIC00170
C                                                                                 FIC00180
C  USE C.G.S. UNITS!!!!! (CONC==>GCL/CC**3)                                       FIC00190
C                        (TEMP==>DEGREES K)                                       FIC00200
C                                                                                 FIC00210
C  BULK FLUID PROPS                                                               FIC00220
      OINT = 197.0                                                                FIC00230
      USUP = 79.0                                                                 FIC00240
      U = OINT                                                                    FIC00250
      RHO = 9.5 D-4                                                               FIC00260
      CP = 0.25                                                                   FIC00270
C  RXATE CONSTANT PARAMS                                                          FIC00280
      EKO = 4.5 08                                                                FIC00290
      GG = 1.2 04                                                                 FIC00300
C  HEAT OF REACTION                                                               FIC00310
      DELH = 2.4 05                                                               FIC00320
C  THE 'RATE' FUNCTION DEFINED VIA EFFECTIVENESS FACTOR AND                       FIC00330
C     INTRINSIC KINETICS.  SEE DEF'N IN ROUTINE BELOW.                            FIC00340
      OSCAT = 0.001                                                               FIC00350
      HF = 3.6                                                                    FIC00360
      OF = 0.6                                                                    FIC00370
      VPSP = OF/6.0                                                               FIC00380
C  BED PROPERTIES                                                                 FIC00390
      EBED = 0.40                                                                 FIC00400
      OSUF = 3.5                                                                  FIC00410
      DIST = OSUF / EBED                                                          FIC00420
      DIFFE = OSUF                                                                FIC00430
      CONDE = 0.00152                                                             FIC00440
C  FILM H.T. COEFFS                                                               FIC00450
      HF = .0026                                                                  FIC00460
C  SET HF=0 FOR ADIABATIC REACTOR                                                 FIC00470
      HF = 0.0                                                                    FIC00480
CCC   HF = .0025                                                                  FIC00490
C  INLET CONDITIONS                                                               FIC00500
      CIN = 2.0 D-7                                                               FIC00510
      TIN = 600.0                                                                 FIC00520
C  WALL TEMPERATURE                                                               FIC00530
      TWALL = TIN                                                                 FIC00540
      WRITE(6,2010) HF, TWALL                                                     FIC00550
C  NUMERICAL INTEGRATION PARAMETERS                                               FIC00560
      ROIY = 5.0                                                                  FIC00570
      ZS = 0.5*DT/ROIY                                                            FIC00580
      ZL =  0.10                                                                  FIC00590
      NWIDE = ROIY + 1                                                            FIC00600
      IMAX = 100.0                                                                FIC00610
C  ZWRITE==>DELTA-Z AT WHICH TO WRITE RESULTS...                                  FIC00620
      ZWRITE = 1.0-ZL                                                             FIC00630
C  INITIALIZE PROFILES                                                            FIC00640
      DO 50 I=1,NWIDE                                                             FIC00650
      CCLD(I) = CIN                                                               FIC00660
      TOLO(I) = TIN                                                               FIC00670
50    CONTINUE                                                                    FIC00680
      Z = 0.0                                                                     FIC00690
C                                                                                 FIC00700
C  CALC UNCHANGING PARTS OF A,B,C MATRICES (FOR CRANK-NICHOLS METHOD)             FIC00710
C     ALPHA==>DIFFE FOR CONC ... CONDE FOR TEMP                                   FIC00720
C     B(MAX)==>1 FOR CONC ... (1+GAMMA) FOR TEMP                                  FIC00730
C                                                                                 FIC00740
      B(1) = 0.0                                                                  FIC00750
      C(1) = -1.0                                                                 FIC00760
      E(1) = 0.0                                                                  FIC00770
      NAI = NWIDE - 1                                                             FIC00780
      ITS = 0.5/(ZS**2S)                                                          FIC00790
      DO 100 I=2,NAI                                                              FIC00800
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      ZI = I-1                                                          FIC00810
      A(I) = XIZ * (0.5/ZI - 1.0)                                       FIC00820
      C(I) = -1.0 * XIZ * (0.5/ZI + 1.0)                                FIC00830
100   CONTINUE                                                          FIC00840
      A(NWIDE) = -1.0                                                   FIC00850
C                                                                       FIC00860
C  START LOOP FOR MARCHING DOWN REACTOR                                 FIC00870
      ZPRINT = 0.0                                                      FIC00880
250   CONTINUE                                                          FIC00890
      Z = Z + ZL                                                        FIC00900
      ZPRINT = ZPRINT + ZL                                              FIC00910
      IF(ZPRINT .LT. ZWRITE) GOTO 255                                   FIC00920
      WRITE(6,2020) Z                                                   FIC00930
      WRITE(6,2030)                                                     FIC00940
255   CONTINUE                                                          FIC00950
C  CONCENTRATION                                                        FIC00960
      A(NWIDE) = -1.0                                                   FIC00970
      B(NWIDE) = 1.0                                                    FIC00980
      E(NWIDE) = 0.0                                                    FIC00990
      E(1) = 0.0                                                        FIC01000
      B(1) = 1.0                                                        FIC01010
      C(1) = -1.0                                                       FIC01020
      II = 0/ZL - DIFFS/(ZS*ZS)                                         FIC01030
      XI = 0/ZL + DIFFS/(ZS*ZS)                                         FIC01040
      ESOLT = (1.0-ESED)/ZSED                                           FIC01050
      CCALL(1) = C(1)                                                   FIC01060
      BAX = NWIDE - 1                                                   FIC01070
      DO 300 I=2,BAX                                                    FIC01080
      ACALL(I) = DIFFS*A(I)                                             FIC01090
      CCALL(I) = DIFFS*C(I)                                             FIC01100
      B(I) = XI                                                         FIC01110
      E(I) = -1.0*ESOLT * RATE( TOLD(I), COLD(I), LIMIT)                FIC01120
300   E(I) = E(I) - ACALL(I)*COLD(I-1) + II*COLD(I) - CCALL(I)*COLD(I+1) FIC01130
      CONTINUE                                                          FIC01140
      ACALL(NWIDE) = A(NWIDE)                                           FIC01150
C                                                                       FIC01160
C  NOW, GET SOLUTION VECTOR                                             FIC01170
CCC   WRITE(6,3000) (COLD(I),I=1,NWIDE)                                 FIC01180
      CALL TRIDAG(ACALL, B, CCALL, E, NWIDE, COLD, CHEN)                FIC01190
CCC   WRITE(6,3000) (CHEN(I),I=1,NWIDE)                                 FIC01200
C                                                                       FIC01210
C  TEMPERATURE                                                          FIC01220
      GAMMA = HR/CONDR * ZR                                             FIC01230
      E(1) = 0.0                                                        FIC01240
      B(1) = 1.0                                                        FIC01250
      C(1) = -1.0                                                       FIC01260
      E(NWIDE) = 1.0 + GAMMA                                            FIC01270
      RHOCP = RHO*CP                                                    FIC01280
      B(NWIDE) = GAMMA*TCALL * RHOCP                                    FIC01290
      CCALL(1) = C(1)                                                   FIC01300
      II = 0/ZL - CONDR/(ZR*ZR)                                         FIC01310
      XI = 0/ZL + CONDR/(ZR*ZR)                                         FIC01320
      DO 350 I=1,NWIDE                                                  FIC01330
      TCALL(I) = TOLD(I)*RHOCP                                          FIC01340
350   CONTINUE                                                          FIC01350
      BAX = NWIDE -1                                                    FIC01360
      DO 400 I=2,BAX                                                    FIC01370
      ACALL(I) = CONDR*A(I)                                             FIC01380
      B(I) = XI                                                         FIC01390
      CCALL(I) = CONDR*C(I)                                             FIC01400
      E(I) = DELH*ESOLT * RATE( TOLD(I), COLD(I), LIMIT)                FIC01410
      B(I) = B(I) - ACALL(I)*TCALL(I-1) + II*TCALL(I)                   FIC01420
      E(I) = E(I) - CCALL(I)*TCALL(I+1)                                 FIC01430
400   CONTINUE                                                          FIC01440
C                                                                       FIC01450
C  GET SOLUTION VECTOR                                                  FIC01460
CCC   WRITE(6,3000) (TOLD(I),I=1,NWIDE)                                 FIC01470
      CALL TRIDAG (ACALL, B, CCALL, E, NWIDE, TCALL, TNEW)              FIC01480
CCC   WRITE(6,3000) (TNEW(I),I=1,NWIDE)                                 FIC01490
C  CONVERT BACK TO REAL TEMPERATURES                                    FIC01500
      DO 450 I=1,NWIDE                                                  FIC01510
      TNEW(I) = TNEW(I)/RHOCP                                           FIC01520
450   CONTINUE                                                          FIC01530
CCC   WRITE(6,3000) (TNEW(I),I=1,NWIDE)                                 FIC01540
C  CALC BULK VALUES, CAT TEMPS, AND RATES.  WRITE RESULTS               FIC01550
C  NO NEED TO DO THIS IF NOT TIME TO PRINT OUT RESULTS                  FIC01560
      IF(ZPRINT .LT. ZWRITE) GOTO 550                                   FIC01570
C  RESET ZPRINT AND THEN WRITE RESULTS...                               FIC01580
      ZPRINT = 0.0                                                      FIC01590
      CSUM = 0                                                          FIC01600
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      TSOR = 0                                                          FIC01610
      RSOR = 0                                                          FIC01620
      RGLO = 0                                                          FIC01630
      DELR = ZR                                                         FIC01640
      DO 500 I=2,NWIDE                                                  FIC01650
      RNEW = RGLO + DELR                                                FIC01660
      AREA = RNEW**2RNEW - RGLO*RGLO                                    FIC01670
      CSOR = CSOR + RNEW*CNEW(I) + RGLO*CNEW(I-1)                       FIC01680
      TSOR = TSOR + RNEW*TNEW(I) + RGLO*TNEW(I-1)                       FIC01690
      RGLOB = RMULT * RATE( TNEW(I),CNEW(I), LIMIT)                     FIC01700
      VOL = AREA * ZL * 3.1416                                          FIC01710
      RGLOB = RGLOB * VOL                                               FIC01720
      TSOL = TCAT( TNEW(I),CNEW(I), LIMIT)                              FIC01730
      WRITE(6,2040)I, CNEW(I), TNEW(I), TSOL, RGLOB                     FIC01740
      RSOR = RSOR + RGLOB                                               FIC01750
C  SAVE OLD VALUES                                                      FIC01760
      RGLO = RNEW                                                       FIC01770
500   CONTINUE                                                          FIC01780
      CBOLR = DELR * CSOR / (DT*DT*0.25)                                FIC01790
      TBOLR = DELR * TSOR / (DT*DT*0.25)                                FIC01800
      RTOT = RSOR                                                       FIC01810
      RRITE(6,2050)CBOLR, TBOLR, RTOT                                   FIC01820
      CONV = 1.0 - CBOLR/CIN                                            FIC01830
      RRITE(6,2060) CONV                                                FIC01840
C                                                                       FIC01850
550   CONTINUE                                                          FIC01860
C  SAVE INTO 'OLD' VECTORS                                              FIC01870
      DO 600 I=1,NWIDE                                                  FIC01880
      CCLD(I) = CNEW(I)                                                 FIC01890
      TOLD(I) = TNEW(I)                                                 FIC01900
600   CONTINUE                                                          FIC01910
      IF(Z .LT. ZMAI) GOTO 250                                          FIC01920
C                                                                       FIC01930
C  FORMATS. . .                                                         FIC01940
2000  FORMAT(5(' *'),' FICK2D FORTRAN',5(' *') )                        FIC01950
2010  FORMAT(' DT=',E13.6,' TWALL(DEG-K)=',E13.6)                       FIC01960
2020  FORMAT(' ------Z (CM) =',E13.6)                                   FIC01970
2030  FORMAT(' I', 5X,'CONC',11X,'TEMP',11X,'TCAT',11X,'RATE(MOL/S)')   FIC01980
2040  FORMAT(I5, 8(2X,E13.6) )                                          FIC01990
2050  FORMAT(' CBOLR=',E13.6,' TBOLR=',E13.6,' TOTAL RATE=',E13.6)      FIC02000
2060  FORMAT(' CONVERSION=',E13.6)                                      FIC02010
C3000  FORMAT(8(2X,E13.6))                                              FIC02020
      STOP                                                              FIC02030
      END                                                               FIC02040
      SUBROUTINE TRIDAG(L,B,C,R,NWIDE,IOLD,INEW)                        FIC02050
      IMPLICIT REAL*8 (A-H,O-Z)                                         FIC02060
C  NOTE--ONLY DIMENSIONED FOR 20 RADIAL DIVISIONS                       FIC02070
C  FOLLOWS FLOW CHART GIVEN BY HORNBECK                                 FIC02080
C  NWID--VECTOR LENGTH                                                  FIC02090
C  OTHER NOTATION--SEE HORNBECK                                         FIC02100
      DIMENSION A(21), B(21), C(21), R(21)                              FIC02110
      DIMENSION IOLD(21), INEW(21), AA(21), BB(21)                      FIC02120
      A(1) = 0.0                                                        FIC02130
      C(NWIDE) = 0.0                                                    FIC02140
      DO 50 I=1,NWIDE                                                   FIC02150
      AA(I) = A(I)                                                      FIC02160
      BB(I) = B(I)                                                      FIC02170
      INEW(I) = IOLD(I)                                                 FIC02180
50    CONTINUE                                                          FIC02190
      AA(NWIDE) = AA(NWIDE)/B(NWIDE)                                    FIC02200
      BB(NWIDE) = BB(NWIDE)/B(NWIDE)                                    FIC02210
C  CALC INTERMEDIATE VARIABLES                                          FIC02220
      DO 100 I=2,NWIDE                                                  FIC02230
      J = NWIDE - I + 2                                                 FIC02240
      TEMP = 1.0/( B(J-1) - AA(J)*C(J-1) )                              FIC02250
      AA(J-1) = AA(J-1) * TEMP                                          FIC02260
      BB(J-1) = ( BB(J-1) - C(J-1)*BB(J) )*TEMP                         FIC02270
100   CONTINUE                                                          FIC02280
C                                                                       FIC02290
C  NOW, SOLUTION VECTOR                                                 FIC02300
      INEW(1) = BB(1)                                                   FIC02310
      DO 200 I=2,NWIDE                                                  FIC02320
      INEW(I) = BB(I) - AA(I)*INEW(I-1)                                 FIC02330
200   CONTINUE                                                          FIC02340
      RETURN                                                            FIC02350
      END                                                               FIC02360
      FONCTION RATE(T,C,LIMIT)                                          FIC02370
      IMPLICIT REAL*8 (A-H,O-Z)                                         FIC02380
      COMMON /BLK/ DECAT, VPSP, DELR, NP, ZKO, GG, CIN                  FIC02390
C  CALC SOLID TEMP FROM LINEARIZED FORM                                 FIC02400
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      TSCL = TCAT(T,C,LIMIT)                                            FIC02410
      IF( C .GT. (0.001*CIN)) GOTO 50                                   FIC02420
      RATE = 0                                                          FIC02430
      GOTO 1000                                                         FIC02440
50    CONTINUE                                                          FIC02450
      IF(LIMIT .NE. 0)GOTO 100                                          FIC02460
C  THIS SECTION FOR NO DIFFUSION LIMITATIONS...                         FIC02470
      RATE = C * IK(TSOL)                                               FIC02480
      GOTO 1000                                                         FIC02490
100   CONTINUE                                                          FIC02500
      RATE = (C/VPSP) * DSQRT( DECAT*IK(TSOL) )                         FIC02510
1000  RETURN                                                            FIC02520
      END                                                               FIC02530
      FUNCTION TCAT(T,C,LIMIT)                                          FIC02540
      IMPLICIT REAL*8 (A-H,O-Z)                                         FIC02550
      COMMON /KIN/ DECAT, VPSP, DELH, HP, ZKO, GG, CIN                  FIC02560
      IF(C .GT. (0.01*CIN))GOTO 30                                      FIC02570
      DELT = 0.0                                                        FIC02580
      GOTO 200                                                          FIC02590
30    CONTINUE                                                          FIC02600
      IF(LIMIT .NE. 0)GOTO 40                                           FIC02610
C  THIS SECTION FOR NO DIFF'N LIMITATIONS                               FIC02620
      XI = DELH * IK(T) * C * VPSP                                      FIC02630
      XI = HP / XI                                                      FIC02640
      YI = GG/(T**2)                                                    FIC02650
      DELT = 1.0/(XI-YI)                                                FIC02660
C  TEST SMALL DELTA-T FOR TEST CASE                                     FIC02670
CCC   DELT = 2.0                                                        FIC02680
CCC   GOTO 50                                                           FIC02690
40    CONTINUE                                                          FIC02700
      XI = DELH * C * DSQRT( DECAT*IK(T) )                              FIC02710
      XI = HP/XI                                                        FIC02720
      YI = GG**0.5/(T**2)                                               FIC02730
      DELT = 1.0/(XI-YI)                                                FIC02740
50    CONTINUE                                                          FIC02750
      IF(DELT .GT. 0.0)GOTO 200                                         FIC02760
C  HAVE STABILITY (OR LINEARIZ) PROBLEMS IN HERE...                     FIC02770
      WRITE(6,100)                                                      FIC02780
100   FORMAT('-----PGM ABORT IN FUNC -TCAT- ---',/,                     FIC02790
     1 ' ---- STABILITY OR LINEARIZ PROBLEMS!!!!!!')                    FIC02800
      STOP                                                              FIC02810
200   CONTINUE                                                          FIC02820
      TCAT = T + DELT                                                   FIC02830
      RETURN                                                            FIC02840
      END                                                               FIC02850
      FUNCTION IK(T)                                                    FIC02860
      IMPLICIT REAL*8 (A-H,O-Z)                                         FIC02870
      COMMON /KIN/ DECAT, VPSP, DELH, HP, ZKO, GG, CIN                  FIC02880
      IK = ZKO / DEXP( GG/T )                                           FIC02890
      RETURN                                                            FIC02900
      END                                                               FIC02910
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I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.

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